December 2004

Science & Technology REVIEW

National Nuclear Security Administration's
Lawrence Livermore National Laboratory

Diamonds Put the Squeeze On Materials

Also in this issue:

- **Predicting the Structure of Proteins**
- **Simulations Show Fluids in Motion**
- **A Closer Look at High-Explosive Detonations**

About the Cover

Livermore scientists have modified the diamond anvil cell, a small tool for studying materials under extreme pressures, by embedding tungsten microcircuits in the diamonds. The modified diamonds, called designer diamond anvils, have tiny diagnostic instruments that can be placed close to a sample. Designer diamond anvils can thus directly record data about material properties and provide more accurate measurements of material behavior under varying pressure. Three types of designer diamond anvils are fabricated for Livermore's research: one for high-pressure electrical conductivity experiments (shown on the cover), another for magnetic susceptibility experiments, and a third for electrically heating high-pressure samples to high temperatures. The article beginning on p. 4 describes this innovative technology and how scientists are using it to support the Laboratory's mission in stockpile stewardship.

Cover design: Kitty Madison

About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy's National Nuclear Security Administration. At Livermore, we focus science and technology on ensuring our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published 10 times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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National Nuclear Security Administration

Prepared by LLNL under Contract No. W-7405-Eng-48

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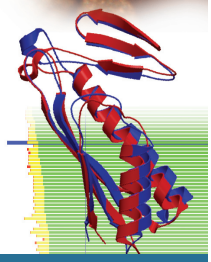

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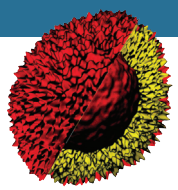

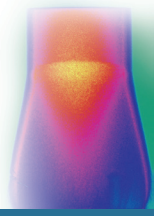

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S&TR, a Director's Office publication, is produced by the Technical Information Department under the direction of the Office of Policy, Planning, and Special Studies.

S&TR is available on the Web at www.llnl.gov/str.

Printed in the United States of America

Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161

UCRL-TR-52000-04-12
Distribution Category UC-99
December 2004

Inactive genes may cause bubonic plague

An international team led by researchers at Livermore's Biology and Biotechnology Research Program Directorate has found that the virulence of bubonic plague—whose bacterium is perhaps the most infectious in humans—may be caused by the inactivation of several hundred genes as the bacterium evolved over time. The plague has long been considered a prime candidate for bioterrorism because of its virulence and potential to be spread.

To study the plague bacterium, *Yersinia pestis*, researchers first sequenced the complete genome of *Y. pseudotuberculosis*. This bacterium has an almost identical DNA sequence to *Y. pestis*. However, *Y. pseudotuberculosis* produces distinct and less acute symptoms than *Y. pestis* and, thus, is rarely fatal. Researchers compared the DNA sequences of two *Y. pestis* strains with the *Y. pseudotuberculosis* genome. Although the comparison revealed several genes in the plague bacterium that are not present in its relative, researchers also found that as many as 13 percent of *Y. pestis* genes are inactive.

The research, conducted in conjunction with the Yersinia Research Unit of the Institut Pasteur in Paris and several other organizations, was reported in the September 21, 2004, issue of the *Proceedings of the National Academy of Sciences*. The study suggests that natural selection may have led to the inactivation of genes that tend to suppress the lethality of *Y. pestis*.

Sequencing of the *Y. pseudotuberculosis* genome was part of an initiative funded by the Department of Energy's Chemical and Biological Nonproliferation Program, which is now part of the Department of Homeland Security's Science and Technology Directorate.

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Earth's mantle may provide energy

Researchers have discovered that untapped methane reserves may exist well below Earth's surface and could provide a virtually inexhaustible source of energy for future generations. A team from Lawrence Livermore, Carnegie Institution's Geophysical Laboratory, Harvard University, Argonne National Laboratory, and Indiana University at South Bend reported their findings in the September 28, 2004, issue of the *Proceedings of the National Academy of Science*.

The scientists used a series of experiments and theoretical calculations to demonstrate that methane—the main component of natural gas—forms under the temperatures and pressures that occur in Earth's upper mantle when carbon in calcite combines with hydrogen in water.

Although methane is the most plentiful hydrocarbon in Earth's crust, oil and gas wells are typically drilled only 5 to 10 kilometers beneath the surface. At these depths, the pressure is only a few thousand times the pressure at Earth's surface—not high enough to transform the subsurface materials. Using a diamond anvil cell, the scientists squeezed materials common at Earth's surface—iron oxide, calcite, and water—to pressures from 50,000 to 110,000 atmospheres (5 to 11 gigapascals) and temperatures to above 1,300°C, creating conditions similar to those found deep within Earth. In these experiments, methane was produced over a range of temperatures and pressures. Production was most favorable at 480°C and 70,000 atmospheres of pressure. Above 1,200°C, the carbon in calcite formed carbon dioxide instead of methane.

These experiments indicate that hydrocarbons may be created from nonbiological reactions between water and rock, not just from the decomposition of living organisms. Because calculations show that methane is thermodynamically stable under conditions typical of Earth's mantle, scientists believe methane reserves could potentially exist for millions of years.

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Simulations point to unexpected physics in hydrogen

Livermore scientists have used quantum simulations to compute the melting temperature of hydrogen as a function of pressure. Their results indicate that the melting curve of hydrogen has a maximum, which opens up the interesting possibility of finding a low-temperature metallic fluid at about 4 million atmospheres of pressure (400 gigapascals). Such a fluid is expected to have unusual properties and would likely represent an entirely new state of matter.

In addition to predicting the melting curve, the simulations provide a microscopic model showing the physical origin of the maximum melting temperature in hydrogen. Contrary to previous expectations, the researchers have discovered that the hydrogen melting temperature is strongly influenced by subtle changes in intermolecular interactions that occur in the fluid phase at ultrahigh pressure.

Numerous experiments have attempted to measure the high-pressure phases of hydrogen. However, until now, the phase boundary that separates the solid and liquid phases has remained relatively unknown. With this new understanding of the physical process involved in the melting of hydrogen, the Livermore researchers have proposed experiments to measure the solid–liquid phase boundary. Results from the team's research appeared in the October 7, 2004, issue of *Nature*.

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Weapons Research Provides a Remarkable Tool for Basic Science

THE Department of Energy's Stockpile Stewardship Program is central to Livermore's national security mission. Underlying all of the Laboratory's activities in stockpile stewardship is a commitment to ensuring that nuclear weapons will continue to be safe and reliable. As part of these efforts, Livermore researchers work to improve the ability to model the behavior of energetic materials (chemical high explosives) and metals at extreme conditions. In particular, they are focusing on how nuclear weapons materials, such as plutonium and uranium, behave under high pressures and temperatures.

The explosion process of a nuclear weapon produces interesting phase changes. The only other environment where such extreme pressure and temperature conditions occur is in the center of big planets, such as Jupiter and Neptune. At Livermore, our stockpile stewardship responsibility requires that our researchers have the tools they need to duplicate such conditions in a laboratory setting.

As the article beginning on p. 4 describes, the diamond anvil cell (DAC) requires only a microgram of material and allows Livermore researchers to study plutonium under extreme pressures without an explosion. Fifteen years ago, geologists used laser-heated diamond anvils to study the phase changes that occur in iron when it is under the temperatures and pressures at Earth's core. Livermore researchers believed the same technology could help them understand where and when plutonium melts in a nuclear weapon. The importance of knowing when these state changes occur can be illustrated with an ice-skating analogy. Before ice skaters venture onto a lake on a warm day, they must determine whether the lake is frozen or the ice is melting. Likewise, in taking care of a stockpile, we must know when plutonium is liquid and when it is solid.

Until recently, it has been very difficult, even with a DAC, to perform electrical conductivity and magnetic susceptibility studies because of the challenge involved in placing diagnostic equipment close enough to the tiny samples to record accurate measurements. To solve this problem, Livermore researchers developed a new type of designer diamond anvil by embedding tiny tungsten coils into the diamonds. The coils are microcircuits that allow scientists to measure material properties under static pressure and then vary pressures and temperatures to simulate conditions occurring in a nuclear weapon.

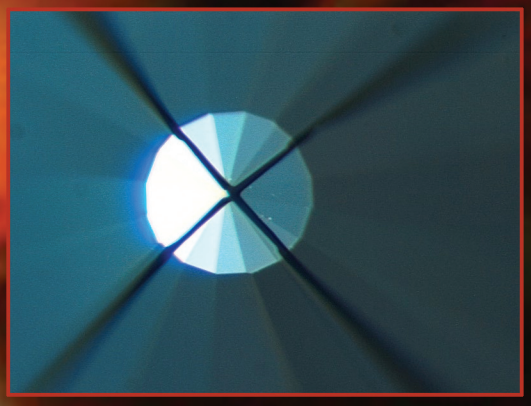
Today, we can develop simulation codes that more accurately reflect changes in a nuclear weapon because the designer DAC provides direct access to what is going on inside the weapon. When weapon scientists relied on underground nuclear testing to supply experimental data on plutonium, they could only infer the metal's state changes. Our understanding of these processes now is so radically different from what we thought occurred in a weapon 15 years ago that I could never then have imagined that we would be where we are today.

Livermore's advances with DACs also illustrate the importance of the Laboratory Directed Research and Development (LDRD) Program. Applying DACs to study plutonium was beyond the scope of the ongoing weapons program, but LDRD support helped launch their use for this weapons-related application. That risk taken 15 years ago turned out to have a huge payoff.

This work is a classic example of how research within the context of the nuclear weapons program produces fundamental science that is remarkable in its own right. Usually, fundamental scientific discoveries help to advance applied science. In this case, applied science produced a tool for pure science. The result is improved precision of computer codes to model weapon performance, which helps ensure the safety and reliability of the nation's aging nuclear weapons stockpile. In addition, that same applied science advances basic science in many other areas, helping scientists improve their understanding of the universe.

■ Bruce T. Goodwin is associate director of Defense and Nuclear Technologies.

Putting the Squeeze on Materials



A new type of diamond anvil cell encapsulates tiny wires in a thin diamond film to reveal information about materials' behavior under high pressure.

FEW gemstones are as mesmerizing as diamonds. Livermore physicists also find diamonds attractive but for reasons other than their beauty. The researchers use flawless, polished diamonds in opposing pairs, or anvils, to slowly compress samples of materials at extreme pressures. This device, called a diamond anvil cell (DAC), forces materials to reveal new information about how their structure and electrical and magnetic properties change—sometimes drastically—in response to increasing pressure.

A DAC is a small mechanical press that forces together the small, flat tips (called culets) of two brilliant-cut diamond anvils. The diamond tips press on a microgram sample of a material, held within a metal gasket, to create extremely high pressures. Diamonds are used because they are the hardest known solid and so can withstand ultrahigh pressures. They also permit diagnostic radiation, such as x rays and visible light, to pass unhampered through their crystalline structure.

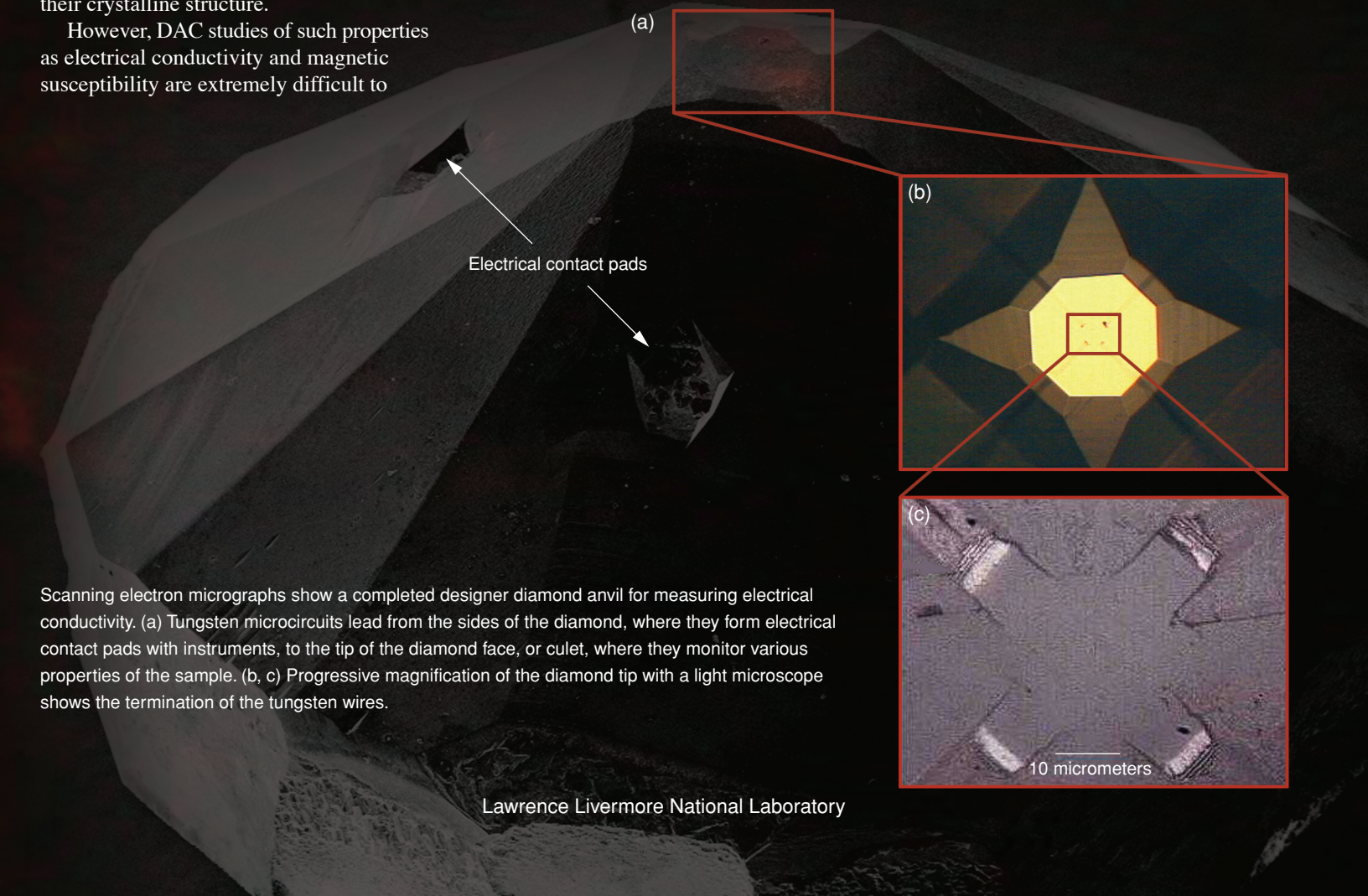
However, DAC studies of such properties as electrical conductivity and magnetic susceptibility are extremely difficult to perform. The 1-microgram samples have a diameter of about 75 micrometers, and diagnostic instruments cannot be placed close enough to them to make the required measurements. Problems especially arise when researchers try to obtain information about materials at static pressures above 1 million atmospheres, or 100 gigapascals (GPa). (For comparison, the atmospheric pressure at sea level is about 1/10,000th of 1 GPa, and the pressure at the center of Earth is about 3.6 million atmospheres.)

To overcome the problems posed by standard diamond anvils, Livermore researchers have taken advantage of recent improvements in diamond synthesis technology to fabricate microcircuits within the diamond anvils themselves. The tungsten microcircuits serve as tiny diagnostic instruments that measure data about materials' fundamental physical and mechanical properties under high pressures. The researchers call this modified tool a designer diamond anvil because the microcircuits can be altered to suit the needs of the experimenter.

Pressuring Materials to Change

Materials behave quite differently under extreme pressures than they do at normal atmospheric pressure. Oxygen, for example, becomes a shiny metal under ultrahigh pressure. In support of the National Nuclear Security Administration's Stockpile Stewardship Program, Livermore researchers are particularly interested in better understanding how nuclear weapon materials, such as plutonium and uranium, behave under high pressures.

Experiments with DACs provide stockpile stewardship data that complement data from shock experiments and tests driven by high explosives. All of these data improve the precision of computer codes that scientists use to model weapon performance and thus, help to ensure the safety and



Scanning electron micrographs show a completed designer diamond anvil for measuring electrical conductivity. (a) Tungsten microcircuits lead from the sides of the diamond, where they form electrical contact pads with instruments, to the tip of the diamond face, or culet, where they monitor various properties of the sample. (b, c) Progressive magnification of the diamond tip with a light microscope shows the termination of the tungsten wires.

reliability of the nation's aging nuclear weapons stockpile. In particular, experimental data are used to refine a material's pressure–volume–temperature relationship (its equation of state, or EOS) and the resulting structural changes (its phase diagram).

With DACs, researchers can measure material properties directly under static pressure, and they can vary pressures and temperatures slowly over the course of many hours. Livermore scientists are using designer DACs to learn how high pressures cause materials to change their magnetic properties, switch from insulators to metals, and alter their molecular structures.

"It is difficult to learn about electrical conductivity and magnetic properties with standard diamond anvils at high pressures," says Livermore physicist and designer anvil inventor Sam Weir. "Until recently, we were limited to trying to maneuver wires into place with tweezers, but these wires deform, break, and short-circuit. Our approach now is to build tiny tungsten wires inside the diamonds so they survive the high pressures. We lithographically fabricate thin-film wires on top of the anvil and then 'grow' a layer of diamond on top of the wires to protect them."

Designer Diamonds Hand-Fashioned

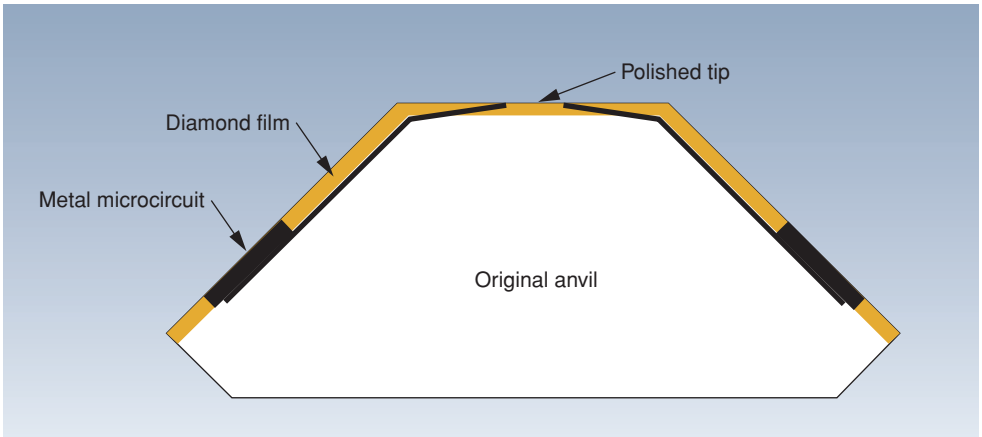
Every designer diamond anvil is custom-fabricated by researchers from Livermore and the University of Alabama at Birmingham. (See the box on p. 8.) The production team makes three types of designer diamond anvils: one for high-pressure electrical conductivity experiments, another for magnetic susceptibility experiments, and a third for electrically heating high-pressure samples to high temperatures. Each type features a unique pattern of microcircuits, usually made of tungsten, which are fabricated on the diamond tip and then encapsulated within a diamond film. These microcircuits terminate on the diamond's sides, where they can be connected to instruments that collect data with high accuracy and sensitivity.

Electrical conductivity experiments use four to eight tungsten wires, magnetic susceptibility experiments require a microloop of about ten turns of wire, and high-temperature experiments use eight wires.

The designer diamond anvil is placed in a beryllium–copper cell about 6 centimeters tall and 3 centimeters in diameter. The cell, in turn, is placed in a small device consisting of a gear-driven piston and cylinder mechanism that can push diamond tips together with a controlled force great enough to generate ultrahigh pressures between the tips. Turning the knob on this mechanism pushes the designer diamond anvil (usually located on the bottom) against a stationary, standard diamond anvil, increasing the pressure and maintaining it indefinitely.

Because diamonds are transparent, scientists can use DACs to make optical and x-ray measurements. Livermore researchers use a light microscope to monitor an experiment. In addition, they place a tiny chip of ruby next to the sample to measure pressure. When green or blue visible laser light shines on the ruby, the ruby emits red light at a wavelength of about 694 nanometers. As the pressure increases, the wavelength increases.

For some experiments, the researchers transport the DAC to a source of very bright, highly collimated x rays, such as the National Synchrotron Light Source at Brookhaven National Laboratory in New York. The scientists pass a beam of x rays through the sample and both diamonds and record the resulting diffraction pattern on an x-ray film or detector. Changes in the diffraction pattern reveal how a material's structure responds to pressure.



A designer diamond anvil uses a one-third-carat diamond. Tungsten metal microcircuits are fabricated on the diamond's 300-micrometer-wide polished tip. These microcircuits are covered with a thin film of diamond and then polished to reveal the tips of the microcircuits on the top of the diamond face.

Focus on Two Element Groups

Many designer DAC experiments focus on two groups of elements—the lanthanides and the actinides—which include the nuclear weapon metals uranium and plutonium. The experiments provide data about lanthanides and actinides that standard DAC techniques and dynamic experiments cannot supply.

Most of the pressure-driven changes the researchers see can be explained by the behavior of a material's electrons. Weir explains that under extreme pressures, certain electrons, which are normally tightly held within an atom's inner electron bands or shells, can move about, resulting

in changes in material properties and molecular structures. In lanthanides and actinides, these electrons belong to an atom's 4f and 5f bands. "Most experiments don't give insight about the cause of volume changes," says Weir. "Our experiments do because we can explain the changes by the delocalization of electrons from specific bands they normally occupy."

How Insulators Become Metals

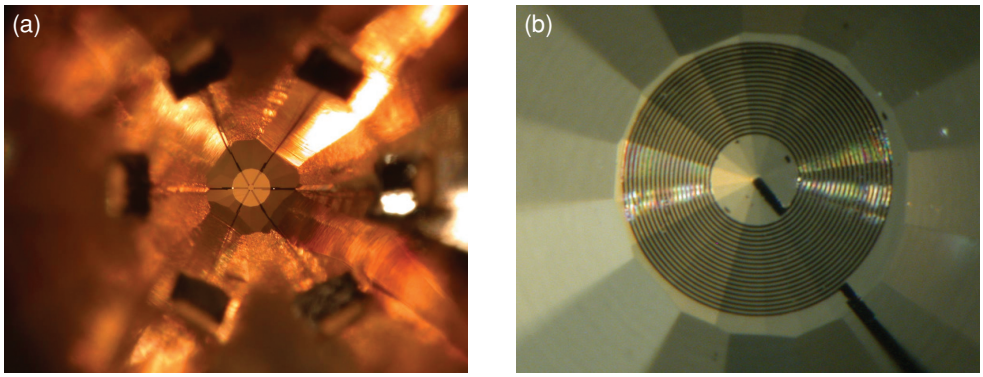
Postdoctoral researcher Reed Patterson performed one of the first experiments with a designer DAC to determine why compounds such as manganese oxide (MnO) are insulators—that is, why they resist the movement of electrons. Electrical conductivity experiments, which probe materials' insulating nature, can only be accomplished at ultrahigh pressures using DACs equipped with designer diamond anvils.

Patterson performed several high-pressure electrical conductivity experiments on a MnO sample. The experiments used a designer diamond anvil with eight tungsten probes measuring 10 micrometers wide and 0.5 micrometer thick. The probes were covered with diamond film and exposed only at the surface near the center of the diamond anvil's culet, where they make contact with the MnO sample.

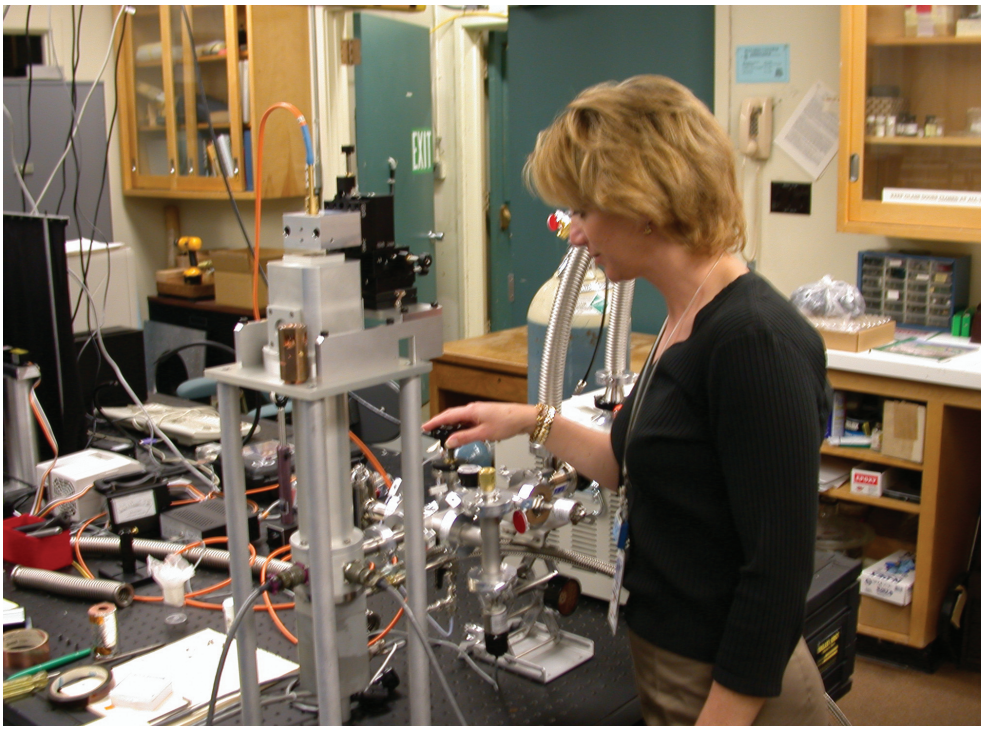
Electrical conductivity was determined by passing a direct current through the wires to the sample and measuring the electrical resistance as a function of pressure. The researchers noted that the sample's electrical resistance rapidly decreased by a factor of 100,000 between 85 and 106 GPa, signaling the transformation of MnO from an insulator to a metal.

The observations provide strong evidence for a pressure-induced insulator-to-metal transition beginning at about 90 GPa, says Weir. "When we squeeze a material, its atoms are forced into a different orientation, which causes the delocalization of electrons. Manganese oxide becomes a metal under these conditions because certain electrons are free to flow instead of staying localized with one atom." The transition is also marked by a nearly 10-percent reduction in the sample's volume, as the crystalline lattice shifts to accommodate the new electronic configuration.

Weir says the results shed light on the high-pressure behavior of other elements with bound electrons, such as lanthanides



Each type of designer diamond anvil features a unique pattern of microcircuits that are fabricated on the diamond tip. A light microscope shows the tip for (a) an electrical conductivity experiment and (b) a magnetic susceptibility experiment.



Livermore scientist Chantel Aracne monitors a high-pressure experiment using a designer diamond anvil cell.

and heavy actinides. Livermore experiments on the lanthanide praseodymium showed that a previously reported 10-percent volume collapse at about 20 GPa coincides with a sudden 60-percent decrease in the metal's resistivity. The sudden drop in resistivity indicates that praseodymium's bound f electrons become delocalized at this pressure. A similar 10-percent volume decrease has been reported in high-pressure experiments on the lanthanide gadolinium at 60 GPa. High-pressure resistivity experiments are under way to investigate whether gadolinium's bound f electrons become delocalized at this pressure.

The researchers are also examining the electrical conductivity of depleted uranium (uranium left over from uranium enrichment processes) at high pressure. They have not discovered significant changes in resistivity that might indicate a change in its electronic or crystallographic structure.

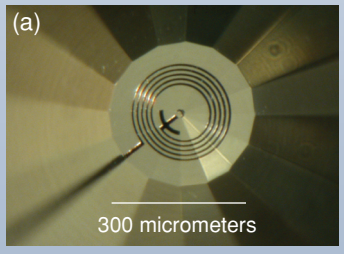
Probing Magnetic Susceptibility

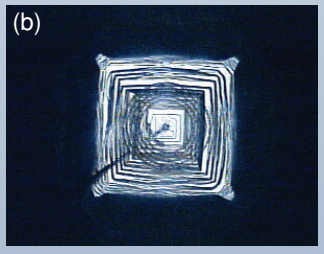
In a project funded by the Laboratory Directed Research and Development (LDRD) Program, Livermore physicists have developed a new type of designer diamond anvil that is equipped with tiny magnetic sensing coils. They are using these

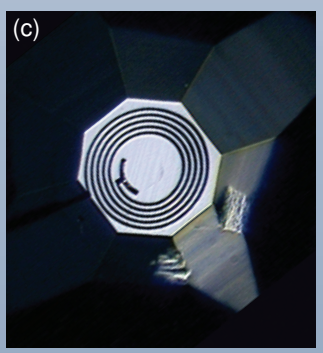
Building a Designer Diamond Anvil

Fabricating a designer diamond anvil is a multistep process that begins with a brilliant-cut, one-third-carat diamond. The diamond's tip must be free of inclusions or defects that could weaken the diamond when it is placed under pressures equivalent to several million times Earth's atmospheric pressure at sea level. At pressures of 100 gigapascals (GPa) and above, the diamonds occasionally shatter into dust. However, at more moderate pressures, they can be reused many times.

The tip of the designer diamond is polished until a flat surface, called a culet, is formed, providing a surface on which the sample can be placed. For experiments at pressures below 50 GPa, the diamond culet ranges from 100 to 500 micrometers in diameter. For experiments above 50 GPa, the culet is beveled downward at the sides so the tip remains relatively flat in response to the pressures.







A designer diamond anvil is made by (a) lithographically fabricating tungsten microcircuits on the diamond's flattened tip, (b) depositing a thin film of diamond over the microcircuits, and (c) polishing the diamond tip so that only the ends of the microcircuits are exposed. This particular designer diamond anvil measures magnetic susceptibility.

Metal microcircuits, or microprobes, made of tungsten are patterned on the tip. Two-dimensional optical lithography, a process used in the semiconductor industry, creates these patterns on the culet. Livermore's three-dimensional laser pantography system, which is managed by Vincent Malba in the Engineering Directorate, is then used to continue the lines on the steep walls of the anvil. Next, a sputtering chamber is used to deposit a thin film of tungsten ions onto the lines of photoresist. Typical probe line widths measure 10 to 30 micrometers. These line patterns extend down the side of the diamond anvil to 125-micrometer-square metal connection points, where leads from external instruments can be connected.

After the tungsten microcircuits are fabricated, a single crystal layer of diamond is deposited on the anvil using a gaseous mixture of 2 percent methane and 98 percent hydrogen. The diamond layer is applied through microwave plasma chemical vapor deposition, a process developed by Vogesh Vohra and Paul Baker at the University of Alabama at Birmingham.

This process lays down a thin film of diamond that varies in thickness from 10 micrometers on the culet to 50 micrometers down the anvil sides. The film is applied at an average rate of 10 micrometers per hour. The film's crystallographic orientation exactly matches that of the substrate. This so-called epitaxial diamond encapsulation is crucial to ensuring that the microprobes survive high pressures.

The rough diamond surface on the anvil's culet is polished to a smooth finish with a tolerance of about 1 micrometer, leaving the microprobes completely encapsulated in diamond except at the tip on the culet and the exposed electrical connectors at the end of the wires on the diamond anvil's sides. These pads make contact with the leads from diagnostic instruments.

Researchers place a 250-micrometer-thick metal gasket on top of the culet. Then they drill a 30- to 150-micrometer-diameter hole in the center of the gasket and place the sample in it. Because diamonds are small, material samples must be the size of pinheads—about 75 micrometers wide. For some experiments, a liquid, gas, or solid is added to the sample to help distribute the compressive force of the diamond faces.

new designer diamond anvils to study the magnetic susceptibility of lanthanides and actinides—that is, how they respond to strong magnetic fields while being subjected to extreme pressures. Data from magnetic susceptibility experiments are expected to improve scientists' understanding of electronic properties and, hence, the different phases of uranium and plutonium.

In the presence of a magnetic field, electrons may align themselves in various ways, much like microscopic bar magnets, or they may not respond at all. Each response reflects the subtle and often competing electron–electron interactions at play in many materials. "Our current understanding of magnetism and magnetic order is far from complete because of electron–electron interactions," says Livermore physicist Damon Jackson, who is leading the experiments.

Magnetic susceptibility experiments with standard DACs are challenging because of the sample's minuscule size and the limitations of sensing coils when they cannot be placed extremely close to the sample. As a result, poor measurement sensitivity and low signal-to-background-noise ratios are common. Designer diamond anvils fabricated for magnetic susceptibility experiments, however, significantly increase data quality because the sensing coils can be placed within a few micrometers of the high-pressure sample.

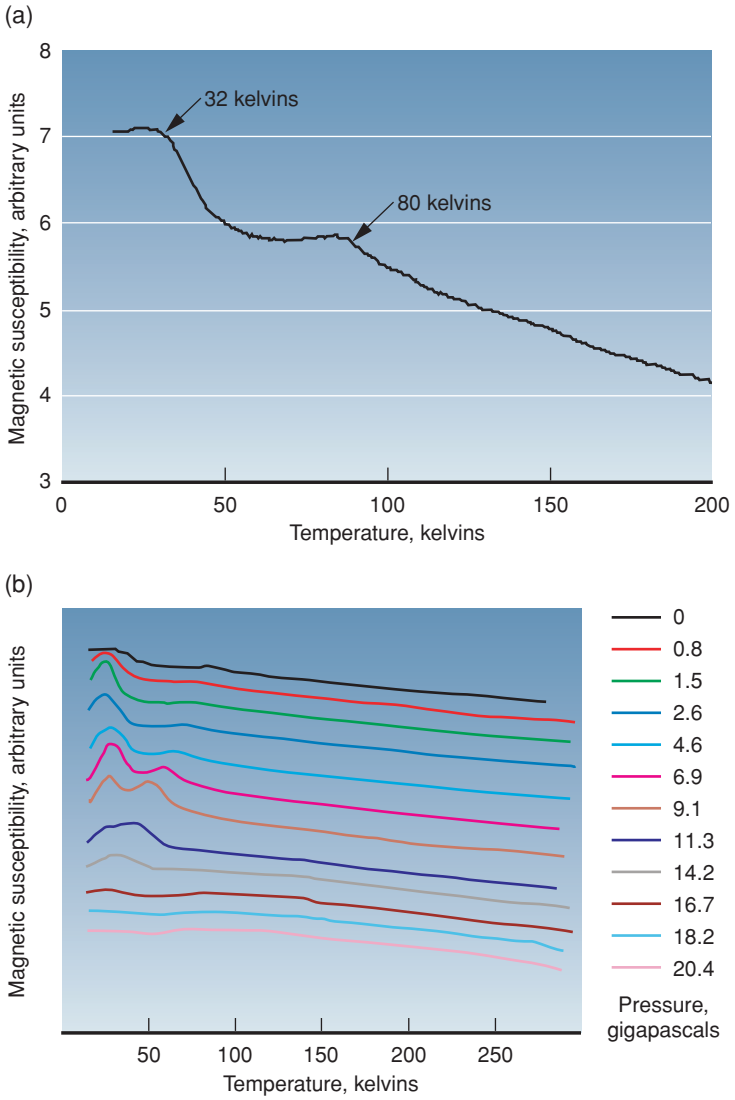
In these experiments, an excitation coil surrounding the sample creates a varying magnetic field. The sample's response is then measured by detecting the voltage induced in a sensing coil embedded in the tip of a designer diamond anvil. Any changes in the magnetic susceptibility of the sample alter the amount of magnetic flux passing through the sensing coil, which results in a change in voltage.

The diamond-encapsulated sensing coil is located just 10 to 20 micrometers below the sample, to increase the sensitivity of the diagnostics. The microcoil typically uses between 10 and 20 turns of tungsten wire (a 20-turn microcoil measures 280 micrometers in outer diameter with a 2.5-micrometer line width). Experiments demonstrated that the microcoils' intrinsic signal-to-background-noise ratio is about 10,000 times higher than with old-style DACs, in which sensing coils are located much farther from the sample.

The excitation coil consists of about 55 turns of copper wire and is wrapped around a standard diamond anvil. The sample, measuring about 75 micrometers in diameter and 50 micrometers thick, is contained within a hole drilled into a metal gasket and sandwiched between the diamond anvils. Typical excitation currents are 10 to 90 milliamperes, which yield magnetic fields up to about 6 gauss. The researchers cool the sample with a helium cryostat to collect magnetic susceptibility data as a function of temperature.

Probing Magnetic Effects

Magnetic susceptibility is a useful probe of f-electron behavior in lanthanides and actinides because the magnetism exhibited in these metals is usually due to their f electrons. High pressures compress the atomic lattice and, thereby, alter the



Experiments with the designer diamond anvil to measure magnetic susceptibility showed two transition states for erbium at room pressure. (a) Erbium's magnetic order is random at room termperature. When it is cooled to 80 kelvins, the magnetic order of its electrons alternates atom by atom. When cooled to 32 kelvins, the electrons from every atom are aligned. (b) Under high pressures, both of erbium's transition temperatures shift in response to the reduced distances between atoms.

magnetic states of the f electrons. Thus, high-pressure magnetic susceptibility experiments provide important physical insights into the electronic interactions affecting the f electrons and, ultimately, the high-pressure EOS of these metals.

When erbium was tested at room pressure, experiments showed two transition states. (See the figure on p. 9.) At room temperature, erbium's magnetic order is random. When it is cooled to 80 kelvins, its electrons become antiferromagnetic; that is, f electrons in alternate atoms show opposite magnetic order. When cooled to 32 kelvins, the sample becomes ferromagnetic, in which all f electrons from every atom are aligned. Under high pressures, both transition temperatures shift in response to changes in the reduced distances between atoms.

Livermore scientists have also conducted magnetic susceptibility experiments on the lanthanides terbium, dysprosium, holmium, and thulium. All show similar magnetic properties in response to temperature and pressure changes.

"We now have an apparatus that can perform highly sensitive magnetic susceptibility experiments on uranium and plutonium samples at extreme pressures," says Jackson. He plans to start experiments on plutonium to characterize its magnetic behavior over a wide range of pressures and temperatures.

Experiments Heat Up

Weir and Jackson recently developed a prototype for yet another type of designer diamond anvil, which uses ohmic heating for experiments at high temperatures and high pressures. This type of designer diamond anvil delivers relatively large amounts of electrical current to the sample and heats it, much like a tiny heating pad would, but to temperatures of thousands of degrees. Six microprobes deliver current for heating, and another two measure the sample's electrical resistance. Sharp changes in resistance indicate phase changes.

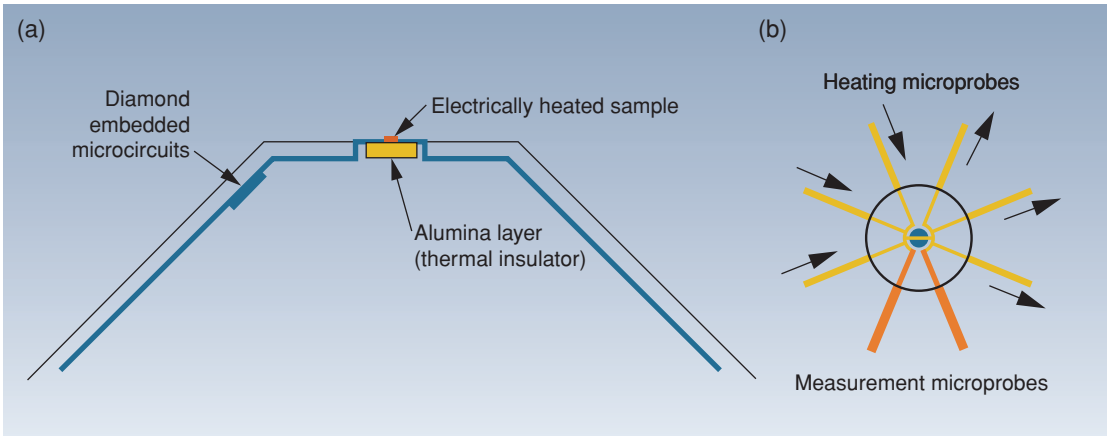
In designing this new type of designer diamond anvil, the physicists had several special requirements to consider. For example, diamond at room temperature has a high thermal conductivity. As a result, using ohmic heating to directly heat a sample to a high temperature is difficult because much of the heat is immediately transferred from the sample to the diamond. To eliminate this problem, the researchers embed the sample in a layer of powdered aluminum oxide (alumina). Using optical lithography and oxygen plasma etching, they excavate a small pit on the culet. The pit, which is 25 micrometers in diameter and about 25 micrometers deep, is packed full of alumina powder, and a sample is placed inside it. As microprobes heat the sample, the alumina-filled pit provides an insulating environment, allowing the sample to withstand significant deformation even at ultrahigh pressures.

Heating experiments on tungsten samples have achieved a maximum of 2,900 kelvins, but adds Weir, "Our heating experiments are just in their infancy."

Looking to the Future

As physicists gain experience in using designer diamond anvils, they are focusing on understanding plutonium under high pressure. In a project funded by LDRD, the researchers are looking for a phase transformation in plutonium at close to 0 kelvin, or absolute zero, the point at which all molecular motion ceases. This phase transformation is called a quantum critical point because near absolute zero, quantum mechanics fluctuations are important and heat fluctuations are not.

Quantum critical points often have important effects at much higher temperatures and could help explain aspects of plutonium's puzzling behavior.



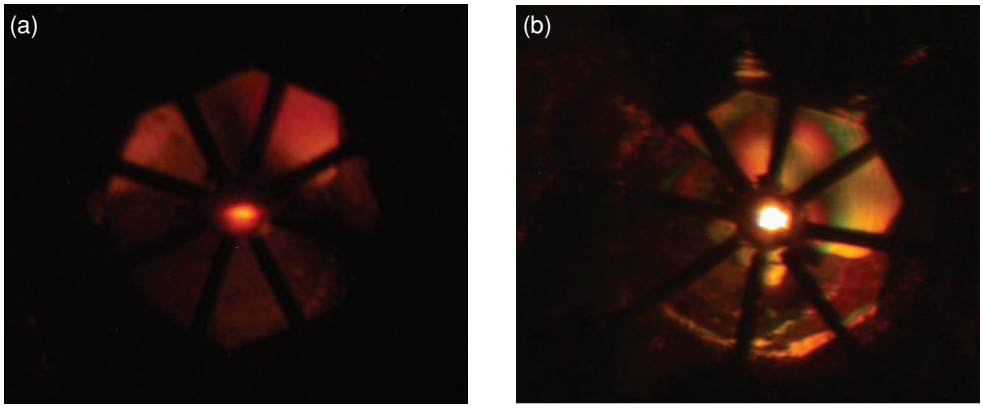
An ohmic-heating designer diamond anvil is used for experiments at high temperatures and high pressures: (a) side view and (b) top view. In this device, six microprobes work to electrically heat the sample, and two microprobes measure its electrical resistance. Because diamond at room temperature has a high thermal conductivity, researchers embed the sample in a layer of powdered aluminum oxide (alumina), which acts as a thermal insulator.

"Plutonium has many structural transitions or phases, which might be the result of a quantum critical point that exists only near 0 kelvin," says Jackson.

Quantum critical points are typically investigated by cooling a material to the lowest practical temperature and then varying a material property, such as chemical composition, or applying a high pressure or a magnetic field. The LDRD project is examining how plutonium behaves in response to changes in temperature, magnetic field, and pressure.

Ohmic-heating experiments to be conducted at Brookhaven are also being planned. "We want to take images of the compression of plutonium's lattice as we elevate pressure and temperature," says Weir. He foresees using two designer diamond anvils in combination for the first time to conduct the plutonium heating experiments: one to heat the sample and another to measure its magnetic susceptibility.

Finally, Weir and Jackson are preparing to begin an ambitious project to use a diamond anvil cell to compress solid hydrogen to more than 300 GPa and study its conductive properties. Livermore researchers were the first to metallize high-temperature fluid hydrogen by using a shock compression technique to squeeze hydrogen to ultrahigh densities. The upcoming effort, funded by LDRD, will attempt to metallize hydrogen at low temperatures, where it is in its solid form. Some scientists consider the search for metallic solid hydrogen to be the Holy Grail of high-pressure physics research.



In heating experiments of tungsten, temperature was increased from (a) 1,200 kelvins to (b) a maximum of 2,900 kelvins, creating a glow in the ultrahot, high-pressure (50-gigapascal) sample.

Ultradense hydrogen has long been the subject of intense experimental and theoretical research because of its fascinating properties. Jackson explains that as the lightest element, hydrogen has large quantum fluctuations, even at 0 kelvin, making it difficult for theorists to accurately predict its properties. Hydrogen's properties have important implications for planetary physics because the interiors of the giant planets Jupiter and Saturn are believed to have cores of dense, metallic hydrogen. Ultradense hydrogen also is of interest to stockpile stewardship. Multiple-shock compression experiments on hydrogen to the metallic state have accelerated the development of new hydrogen EOS models, which are important in studies of inertial confinement fusion and other applications.

William Evans and Choong-Shik Yoo from Livermore's Physics and Advanced Technologies Directorate will join Jackson and Weir in the research project. "This ambitious effort will require pushing designer diamond anvils to new extremes in pressure," says Weir. "But if we're successful, it will result in a significant scientific breakthrough."

The future looks bright for designer DACs. Diamonds may well become a physicist's best friend.

—Arnie Heller

Key Words: actinides, designer diamond anvil, diamond anvil cell (DAC), electrical conductivity, ultradense hydrogen, Laboratory Directed Research and Development (LDRD) Program, lanthanides, laser pantography, magnetic susceptibility, microcircuits, plutonium, uranium.

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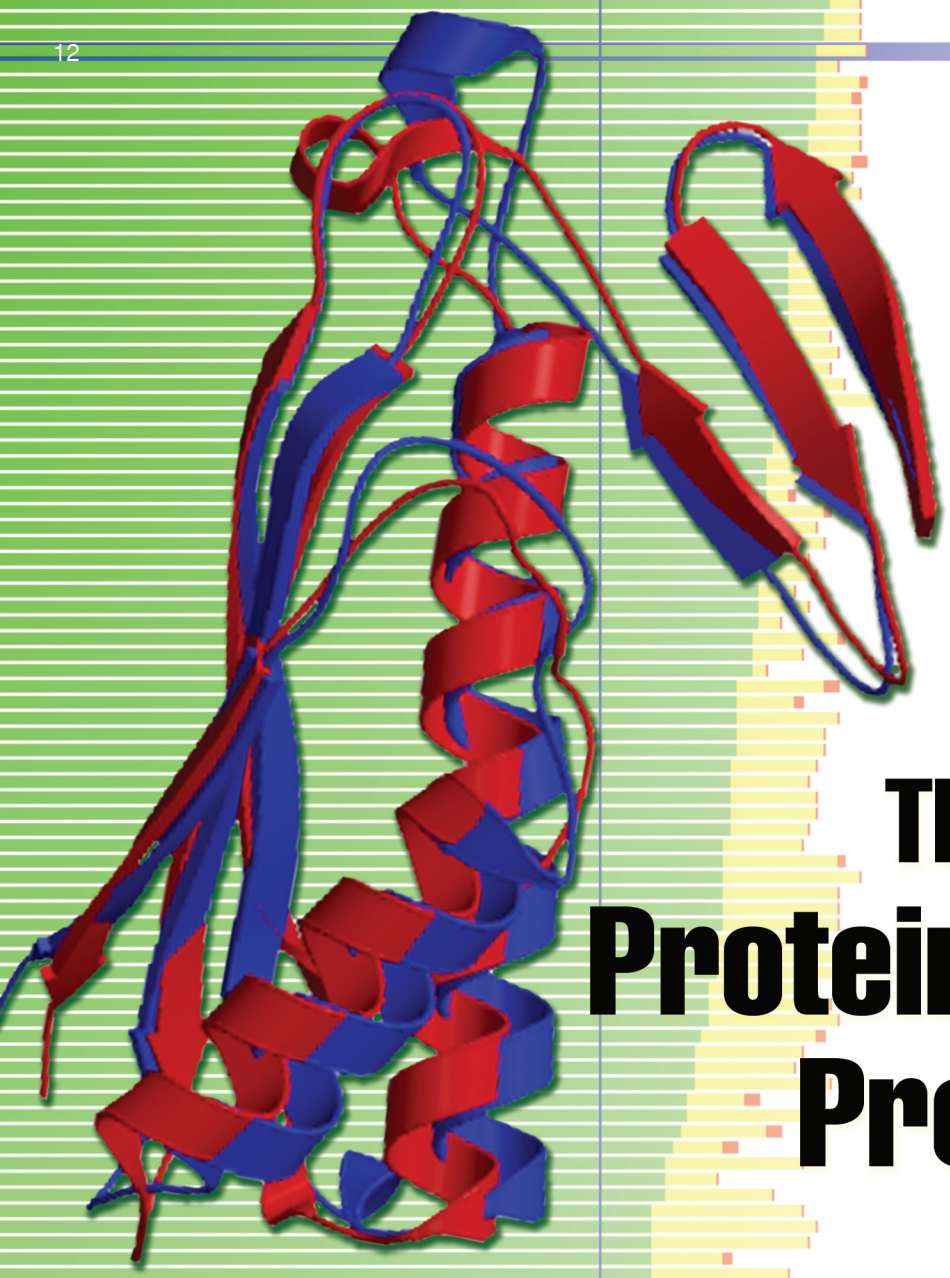


A biennial experiment helps scientists evaluate the best methods for predicting the structures of proteins.

The Art of Protein Structure Prediction

FROM hemoglobin that carries oxygen, to enzymes and hormones that turn cells on and off, to antibodies that fight infection, proteins seem to do it all. There are many different types of proteins, each with a particular shape and function, and those shapes and functions are linked. For example, hemoglobin's shape allows it to carry oxygen; collagen's shape is ideal for connective tissue; and insulin fits in spaces like a key in a keyhole, enabling it to control sugar levels.

Disease can occur when a protein doesn't form, or fold, into its correct shape. Knowing that shape is critical for designing therapeutic drugs, for example, to treat human diseases that result from misfolding. However, predicting

protein shapes remains a daunting scientific challenge.

In 1994, Krzysztof Fidelis, a computational biologist at Lawrence Livermore, and John Moult, a professor at the University of Maryland Biotechnology Institute, received funding from the Laboratory, the Department of Energy (DOE), the National Institutes of Health (NIH), and the National Library of Medicine to organize the Critical Assessment of Techniques for Protein Structure Prediction (CASP). This biennual experiment, which is now funded by NIH with contributions from industry and international agencies, brings together groups of scientists from more than 20 countries with expertise in biology, physics, chemistry, and computer science to predict the structure of proteins.

CASP provides participants with the amino acid sequences for proteins whose structures are close to being determined experimentally by researchers. The participants then submit model structures generated by computer programs for these target proteins. Event assessors compare the prediction models with structures from experimental results.

"For decades, scientists would test modeling techniques using proteins whose structures were already known and think the problem was solved," says Fidelis. "However, the methods would not necessarily work for other structures." CASP allows organizers and participants to gauge which methods are most effective at predicting protein structure. At the sixth conference (CASP6), which is being held in Gaeta, Italy, this month (December 2004), participants will learn which models were most accurate for 76 target proteins.

Solving Structures Experimentally

Predicting the shape into which a protein will fold is difficult because proteins are composed of 20 different amino acids that combine and can adopt one of several trillion shapes. Major steps in understanding the protein puzzle were taken by scientists working on the Human Genome Project, which began as a DOE initiative in 1986 and culminated in 2000 when the DNA sequencing of the entire human genome was completed.

An organism's genome is its full genetic instruction encoded and stored within each cell, providing all of the information the organism needs to maintain and reproduce itself. Each gene carries the instructions for making a particular protein. Once a protein sequence has been determined, experimentalists perform the labor-intensive process of deducing its unique three-dimensional (3D) structure. To help experimentalists determine protein structure more quickly, CASP participants develop computational techniques for predicting structures.

The experimental methods most commonly used to determine a protein's

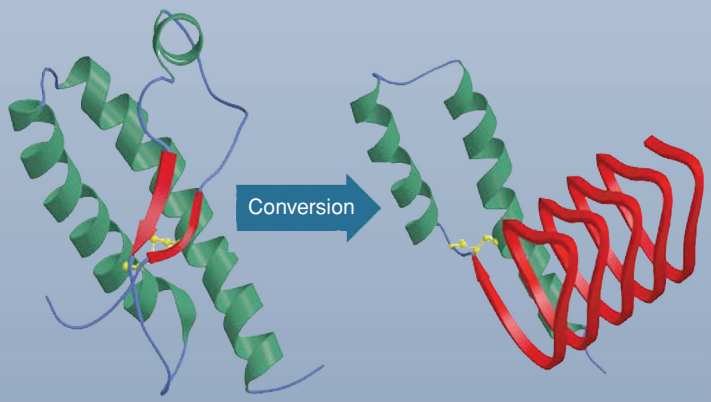
Protein-Folding Diseases

Scientists have identified about 20 diseases caused by protein misfolding, which can be divided into two groups: diseases in which excessive quantities of wrongly folded proteins collect in certain bodily tissues and those in which a correctly folded protein is missing. The most familiar example of the first type is Alzheimer's disease, which afflicts 10 percent of people over 65 years old and half of those over 85. Each year, Alzheimer's kills 100,000 Americans, and about $83 billion is spent to care for its victims.

Another example in this group is the infectious diseases, mad cow and its human form, Creutzfeld–Jakob disease. These conditions seem to occur when normal protein particles called prions misfold. The normal human prion is a component of the membrane of healthy nerve cells that fold and are disposed of without a problem. It can, however, misfold in a particular way that triggers a domino effect in healthy prions, forcing them to adopt its incorrectly folded form.

In the second group of protein-folding diseases, the lack of a correctly folded protein means that too little normally folded protein is available to do the job. This defect is thought to be involved in diseases such as cystic fibrosis, hereditary emphysema, and some cancers.

In the past two decades, scientists have discovered that most cancers result from mutations in the genes that regulate cell growth and cell division. Forty percent of all human cancers involve a gene whose sole function appears to prevent cells with damaged DNA from dividing before the damage is repaired or, if the damage can't be fixed, to induce the cells to destroy themselves. Thus, the key to effective cancer treatment is to design drugs that can either stabilize the normally folded structure or disrupt the pathway that leads to a misfolded protein.



A normal prion resides on the membrane of a nerve cell, where it folds and is disposed of without a problem. In an infected person or animal, the prion misfolds in a manner that triggers healthy prions to adopt the abnormal form.

structure are x-ray crystallography and nuclear magnetic resonance (NMR). In x-ray crystallography, scientists determine protein structure by measuring the directions and intensities of x-ray beams diffracted from high-quality crystals of a purified protein molecule. NMR uses high magnetic fields and radio-frequency pulses to manipulate the spin states of nuclei. The positions and intensities of the peaks on the resulting spectrum reflect the chemical environment and nucleic positions within the molecule. Unfortunately, both methods are expensive and time consuming, and some proteins are not amenable to these techniques.

Scientists have been working to solve the protein-folding mystery for decades. In research that received the 1972 Nobel Prize in Chemistry, Christian Anfinsen showed that a completely unfolded protein could fold spontaneously to its biologically active state, indicating that a sequence of amino acids contains all of the information needed to specify its 3D structure.

Protein molecules—only 3 to 10 nanometers across—can self-assemble quickly, some as fast as a millionth of a second. But this brief period is long for computers to simulate. Two difficulties arise in mimicking the protein-folding process with a computer. "First, the number of possible conformations a protein chain can adopt is too vast to analyze even with today's most powerful computer," says Fidelis. "Second, the estimates of molecular interactions that we use in simulations are simply not accurate enough to render a successful prediction."

Software to Assist Predictors

To help them predict a protein's fold, scientists use computer programs that estimate the molecular forces between all of the protein's atoms and the surrounding molecules. Thus, they try to determine if those forces cause a protein to fold in a certain way. Amino acids respond differently to the watery environment of a living cell. For example, some are drawn to water, while others are repelled by it. Researchers use such characteristics to develop algorithms that help predict structure.

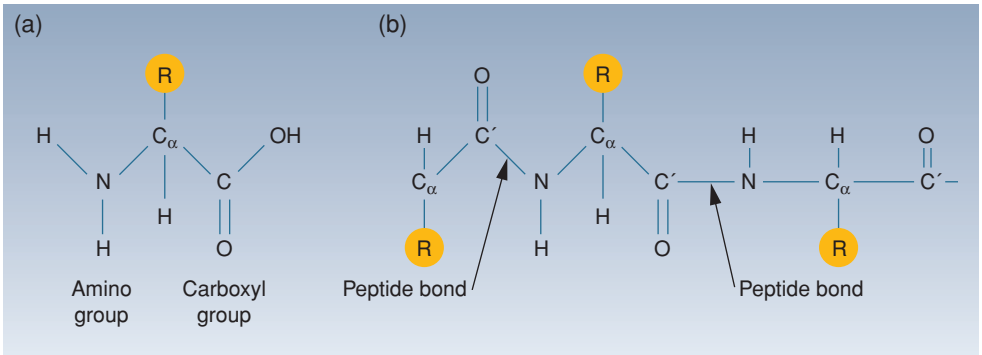
Some prediction programs run molecular dynamics models to calculate the forces between atoms and determine whether those forces would cause the protein to fold a certain way. Other programs cut the protein into smaller sequences and then apply an algorithm that searches for similar protein fragments from the known structures stored in the Protein Data Bank (PDB). Originally developed by DOE's Brookhaven National Laboratory, the PDB is the industry standard for protein structure and currently lists about 25,000 protein structures.

Classifying Structures into Groups

Fortunately for biomedical researchers, there are fewer classes of 3D folds than there are different sequences. In fact, many researchers believe that, because proteins are evolutionarily related, only several thousand unique protein-structure families exist. Livermore computer scientist Adam Zemla explains, "Because there are 20 different amino acids, a medium-size protein with 300 amino acids would theoretically have 20^{300} possibilities in sequence. In nature, not all combinations of amino acids can exist. Scientists estimate that the number of different protein sequences is close to a few million."

All 20 amino acids have a central carbon atom, called carbon-alpha (C_α), to which are attached a hydrogen atom, an amino (NH_2) group, a carboxyl (COOH) group, and a side chain. The side chain distinguishes one amino acid from another. Amino acids join to form peptide bonds when the COOH group of one amino acid joins the amino acid group next to it to eliminate water. This process is repeated as the chain elongates. The repeating units, called residues, are divided into main-chain atoms and side-chain atoms.

The main chain is identical in all residues. It consists of a C_α, to which is attached an NH group, a carbonyl (C´=O) group, and a hydrogen atom. The side-chain atoms are different for each residue and are bound to the C_α. Each amino acid has a different side chain. Some sequences must be so precise that a change of even one amino acid can make a big difference, whereas in other sequences, any amino acid will work. For example, an amino acid change at one position in the protein beta-globin causes sickle cell anemia. (See the box on p 13.)



(a) Each of the 20 amino acids is composed of a central carbon atom, C_α; an amino group, NH_2; a carboxyl group, COOH; a hydrogen atom, H; and a side chain, R, which is different for each amino acid. (b) Amino acids combine to form a polypeptide chain when the carboxyl group has formed a peptide bond, C–N, to the amino group next to it.

Polypeptide chains fold to form a 3D structure, which is composed of one or more regions, called domains. Domains can adopt any combination of three shapes, or secondary structures: alpha helices; beta strands, which combine to form beta sheets; and coils. Secondary structures can serve as modules for building up large assemblies of protein, such as muscle fibers, or they can form binding sites, such as those for enzymes.

Evaluating the Difficulty

The level of difficulty in predicting a protein's structure is determined by the similarity of the protein sequence with that of a known protein structure. Scientists have classified protein-structure prediction methods into three categories. From least difficult to most difficult, they are comparative modeling (CM), fold recognition (FR), and new fold (NF). CM techniques are used when a protein's sequence closely resembles a known protein sequence in the PDB. With CM, the known protein then serves as a template. FR methods compare a specific sequence with all of the known folds in the PDB and estimate the probability of the unknown protein sequence having the same fold as that for a known sequence. NF methods are used when a protein has no detectable structural relative in the PDB. When working on proteins in the NF category, researchers use a combination of techniques to model the folds.

According to Livermore computational biologist Andriy Kryshtafovych, the response to the CASP experiments has been outstanding. "At CASP1, 35 groups submitted 100 predictions for 33 protein targets," says Kryshtafovych. "This year, at CASP6, we have 230 groups submitting more than 41,000 predictions for 76 targets."

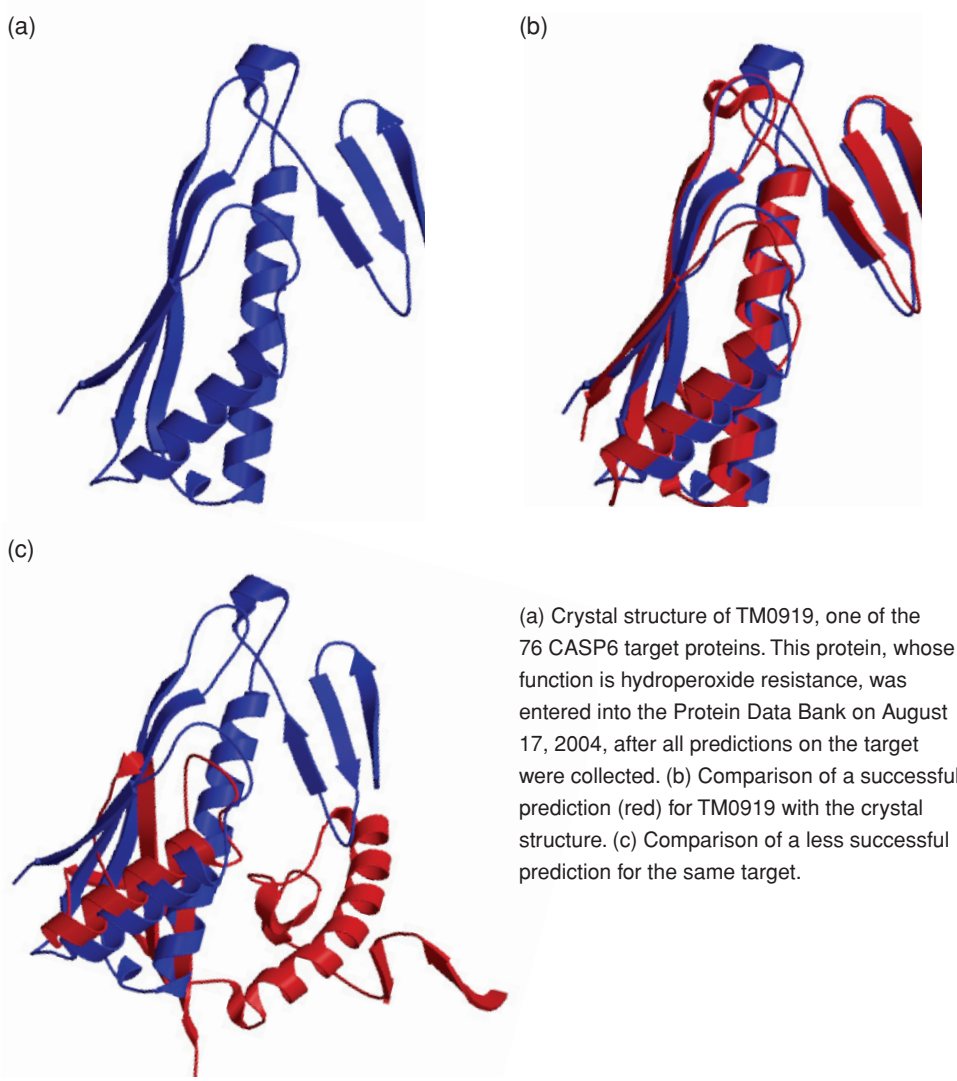
Three independent assessors with expertise in protein folding evaluate the CASP submissions. The assessors determine the category for each target, based on level of prediction difficulty. Then each assessor evaluates submissions in only one category. Assessment is essentially blind—that is, the assessors are not informed of a group's identity or the method used until the submissions are evaluated and scored. An example comparison is shown below.

Groups can submit up to five partial or full predictions for each target. At CASP1, assessors manually evaluated the prediction models—an almost overwhelming task. In 1996, Livermore formed the Protein Structure Prediction Center to develop software tools for streamlining the process. Zemla then designed and developed computer systems that register predictor groups, collect targets, distribute target information to the groups, verify format of submitted predictions, and provide numerical data on submissions to help assessors evaluate them.

"Designing software to evaluate one model isn't difficult," says Zemla. "The challenge is determining which measures are most useful to assessors when evaluating prediction models against each other, especially when two or more partial model predictions for one target do not represent the same piece of the sequence."

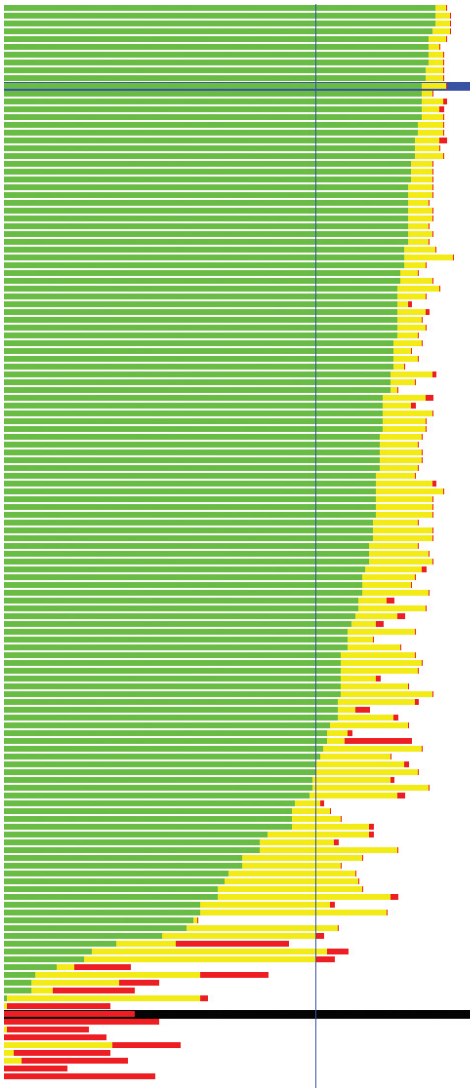
Improving Evaluation Software

Existing model evaluation software uses the root-mean-square deviation (RMSD), a



(a) Crystal structure of TM0919, one of the 76 CASP6 target proteins. This protein, whose function is hydroperoxide resistance, was entered into the Protein Data Bank on August 17, 2004, after all predictions on the target were collected. (b) Comparison of a successful prediction (red) for TM0919 with the crystal structure. (c) Comparison of a less successful prediction for the same target.

standard algorithm that compares distances between a model and a target. The RMSD is an average, so it looks for the best fit where all of the atoms for one set can be superimposed on all of the atoms for the target. However, RMSD has one limitation: When two structures are similar in all but one area, this difference creates a large RMSD, which overstates the dissimilarity between the two structures.



Each bar of this Local–Global Alignment graph represents a prediction for target TM0919. The colors represent the number of amino acid sequences that were correctly aligned (green), closely aligned (yellow), and poorly aligned (red). The predictions shown on p. 15 are highlighted: blue bar = successful model in (b); black bar = poor model in (c).

To resolve this limitation, the Livermore team created a program that searches for local structural similarities between proteins. This method measures similarities between segments of residues rather than calculate the global (all-residues-based) RMSD. Because it allows for slight differences in residue position and focuses on matching segments, the program is better at detecting similar structures than RMSD software.

With funding from the Laboratory Directed Research and Development (LDRD) Program, Zemla also developed a software program called Local–Global Alignment (LGA). The LGA program compares distances between the protein structures for local segments and the global structure. The LGA scoring function has two components: longest continuous segment (LCS) and global distance test (GDT). The LCS algorithm identifies local regions in different proteins where the residues are similar within an RMSD cutoff. The GDT algorithm searches for the largest (but not necessarily continuous) set of equivalent residues from anywhere in the structure that fits with a distance cutoff. (See the figure on p. 17.)

LCS results are generated for a set of increasing RMSD cutoffs—0.1, 0.2, and 0.5 nanometer; for GDT results, the cutoffs range from 0.05 to 1.0 nanometer. These cutoffs are chosen because of the level of certainty in knowing a protein structure with complete accuracy: With x-ray crystallography, the level of certainty is about 0.05 nanometer, and with NMR, it is within 0.10 to 0.15 nanometer. For computer modeling, it may vary more than 0.4 nanometer.

The next challenge for the Livermore team was to convert the vast amount of numerical data generated by the evaluation software into graphics formats that can be displayed on the Web site for the Protein Structure Prediction Center. In evaluating models, assessors use the center's Web site to define the parameters they need, such as RMSD cutoffs or side-chain residue sequences.

Automated Servers Improve Effort

Because of its complexity, protein structure prediction has required researchers to be closely involved in the process. However, a growing number of CASP participants are using automated servers to calculate conformations of protein structure. At CASP4, assessors began evaluating the results from automated servers that were programmed with prediction algorithms. (A parallel organization, the Critical Assessment of Fully Automated Structure Prediction, developed the methods being used to assess the performance of automated servers that do not require human intervention.) At CASP5, FR-category results from the best metaservers were competitive with the best humans.

In the 10 years since the first CASP experiment, the Protein Structure Prediction Center has gathered an enormous amount of data. "For many proteins, especially for difficult targets, the best models are still not accurate enough to be useful for many applications," says Zemla. "The good news is that considerable advances have been made in the NF category and in the automated techniques used on servers."

A Database of Models

Although the quality of predictions hasn't improved as quickly as desired, the results from each experiment are valuable. Prediction models also may prove to be useful in other research areas, such as evolutionary analyses. During the course of evolution, proteins in different organisms have diverged from a common ancestor protein. Changes have occurred in the amino acid sequence of the proteins, but their 3D fold and function have remained the same.

Thus, when two proteins have alignments in which the sequence identity is similar by more than 25 to 30 percent, scientists generally assume that the two sequences have diverged from the same ancestor.

More commonly, however, the sequence similarity has been lost along the evolutionary trail, so comparing structures may be the only way to identify their relationship. "Comparative structural genomics may become a powerful tool to identify the function of proteins and protein systems, helping scientists to better understand the corresponding mechanisms," says Fidelis. "This improved understanding may, in turn, result in better control over engineered modifications that benefit such areas as environmental cleanup or producing therapeutics for human diseases."

In 2003, the Livermore team received LDRD funding to create a database of protein models that will function as both a search tool and a model evaluator. When a protein structure is not found in the PDB, scientists can enter search criteria in the protein model database to look for models that may exist for the structure in question. The team's prototype database currently stores more than 2,000 protein models. Team members are working with their colleagues who maintain the PDB to link the two databases.

Software for Model Evaluation

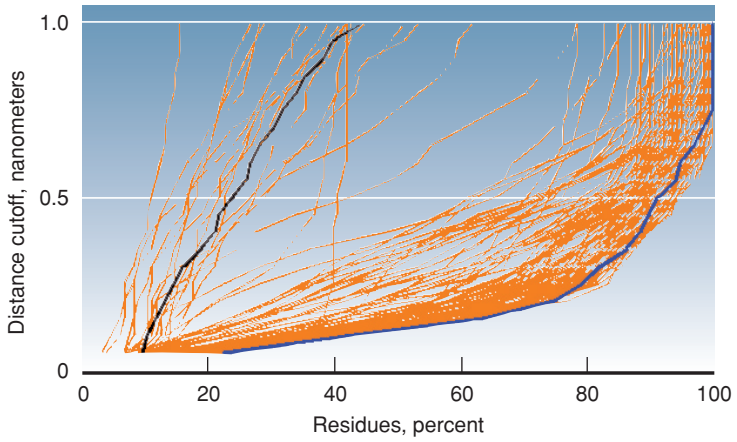
Developing tools to evaluate models is more challenging than developing the database search function. Fidelis explains, "In CASP, we compare the differences between models and a target whose structure is known. It is much more difficult to compare two models that predict a protein whose structure is unknown and determine which one is more accurate." The data collected from CASP may help the team evaluate a method's performance. "We can look at which models came closest to predicting a target's structure in a CASP experiment," says Fidelis, "and then see which method the group used to achieve those results. Some methods work better for CM, some for FR, and others for NF."

Many protein structures are unknown. Groups around the world are all attempting to determine the structures of proteins that are important for current research. The protein model database could help these researchers by combining all of the models to produce a single structural representation that is better than any one model alone.

The Livermore team also plans to use the database in Laboratory projects that study the function of proteins involved in the body's response to infectious disease agents. This application could be particularly useful in support of the Laboratory's national and homeland security missions, for example, helping scientists develop methods to counter a bioterrorist threat.

Just as mapping the human genome led to the rapid discovery of thousands of protein sequences, researchers believe greatly improved protein structure predictions will lead to many discoveries that will benefit virtually every area of life. From designing therapeutics to developing pollution-busting bugs, the possibilities are endless.

—Gabriele Rennie



Results from a global distance test show the percentage of amino acid sequences that each group predicted for one target within the designated distance cutoffs. The blue line represents the successful model shown in (b) on p. 15, and the black line represents the poor model in (c).

Key Words: Critical Assessment of Techniques for Protein Structure Prediction (CASP), global distance test (GDT), Laboratory Directed Research and Development (LDRD) Program, Local–Global Alignment (LGA), Protein Data Bank (PDB), protein folding, Protein Structure Prediction Center.

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On the Web, see predictioncenter.llnl.gov.

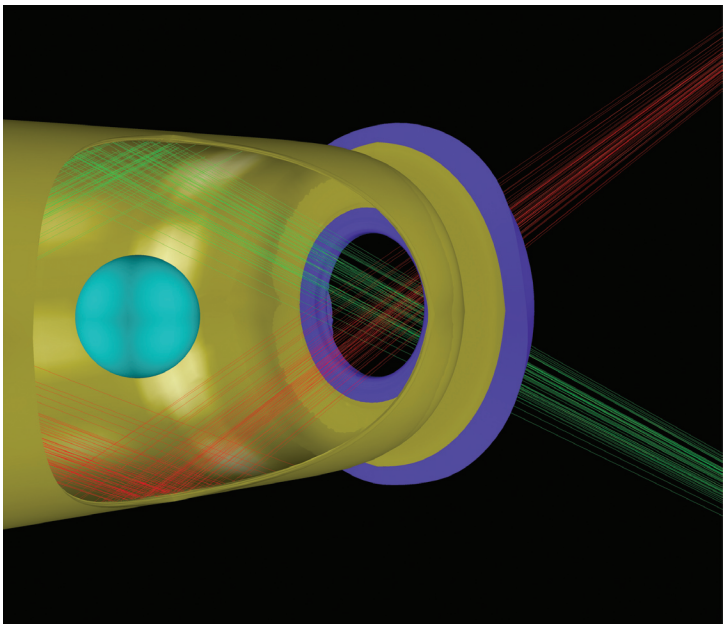
It's All in Motion When Simulating Fluids

WHETHER it's the mechanics of a supernova, the ignition of an inertial confinement fusion (ICF) capsule, or the detonation of a nuclear weapon, simulating the motion of fluids is anything but simple. Every piece of the model is moving. Fluids interact with each other and with solid materials, plus those interactions occur quickly and at intense pressures and temperatures. In some instances, the fluid has almost nothing with which to collide, as happens in simulations of a nuclear explosion in the upper atmosphere or electrons in a fluorescent light bulb.

Scientists in many fields are interested in the motions of fluids. In Livermore's Defense and Nuclear Technologies (DNT) Directorate, researchers study fluid motion to answer questions in astrophysics, atomic and nuclear physics, computational physics, fluid dynamics, turbulence, high-energy-density physics, radiation transfer, and particle transport. Computer scientists work with physicists to write codes that simulate experiments, providing data to augment experimental results or to verify test codes used to predict results in regimes where experiments cannot be performed.

Livermore physicist Jim Rathkopf, who is associate leader for DNT's AX Division, says, "We're looking at a variety of high-energy-density problems related to ICF and national security issues. Many of them require codes with different approaches for modeling the hydrodynamics of gases and plasmas in motion. Our multiphysics codes also simulate physical processes such as radiation, neutron, and charged-particle transport in addition to hydrodynamics."

Three Livermore codes that explore this world of motion are HYDRA, MIRANDA, and CPK. The radiation hydrodynamics code HYDRA is used to help design targets for the National Ignition Facility (NIF). MIRANDA looks at hydrodynamic instabilities, and the complex particle kinetics code CPK bridges the hard-to-model regime between collisionless and collision-dominated plasmas.



Livermore's radiation hydrodynamics code HYDRA was used to simulate a 2-millimeter-diameter ignition target for the National Ignition Facility (NIF). This cutaway view shows representative laser rays from two beams (green, red) as they illuminate the hohlraum wall (gold). Their energy is converted to thermal x rays, which heat the capsule ablator.

Simulating Targets for NIF

When all of NIF's 192 laser beams are operational, they will deliver up to 1.8 million joules of ultraviolet laser energy and 500 terawatts of power to millimeter-size targets. Any asymmetry in how each beam delivers this energy or any perturbation (roughness) on the surface of a target capsule can affect the target's performance. Computational scientists developed HYDRA to evaluate different target designs in realistic three-dimensional (3D) geometries.

The baseline target design for ICF experiments on NIF uses a small metal cylinder, called a hohlraum, surrounding a spherical plastic or beryllium fusion capsule that contains a small amount of deuterium–tritium fuel. When NIF's laser beams simultaneously deposit their energy on the hohlraum's inner surface, much of it is converted to thermal x rays. When the x rays ablate the surface of the capsule, they create a rocketlike effect that causes the capsule to implode, producing high temperatures and pressures in the fusion fuel.

HYDRA can simulate the entire ignition target in 3D, including the hohlraum, capsule, and all relevant features. The code is flexible enough to model intrinsic asymmetries that result from the ideal laser illumination pattern and those that result from effects of irregularities in laser pointing and power balance. It also simulates the hydrodynamic instabilities that occur when the capsule implodes. HYDRA calculates all of the radiation, electron, ion, and charged-

particle transport and the hydrodynamics from first principles—that is, no adjustments are made to the modeling parameters.

These simulations allow scientists to evaluate the robustness of a target design. For example, a designer can place realistic roughness on the capsule surfaces and calculate how these features evolve into irregularities—bubble and spike patterns—as a result of hydrodynamic instabilities. Three-dimensional simulations indicate that the ultimate amplitudes of the bubbles and spikes are greater than are shown in the 2D simulations. Thus, the 3D calculations provide more accurate information on peak amplitudes of these irregularities and how they affect target performance.

HYDRA calculations can now be run on Livermore's Linux-based MCR supercomputing cluster, and with that processing capability, the 7- to 10-day run times have been cut in half compared with run times from a year ago. "For the first time, we can model the entire ignition target in an integrated, 3D simulation," says Livermore physicist Marty Marinak, who leads the HYDRA development team. "We also can resolve the 3D evolution of the full range of interesting Rayleigh–Taylor instability modes. As a result, we have a substantially clearer understanding of how our target designs perform."

Designers are also using HYDRA to evaluate alternative target designs, including one with two concentric spherical shells and direct-drive targets that eliminate the need for a hohlraum. The HYDRA development team continues to enhance the code's capabilities in response to user requests. One new physics package will treat magnetic fields in 3D. Says Marinak, "This addition will enable unprecedented completeness in our modeling and further improve our understanding of the target physics."

Observing Hydrodynamic Instabilities

Another Livermore-developed hydrodynamics code, MIRANDA, is being used to study the behavior of instabilities that evolve when materials of different densities are accelerated. Weapon physicists use MIRANDA simulations to better understand the physics involved in several stockpile stewardship issues they need to address. It also can provide information of interest in astrophysics research.

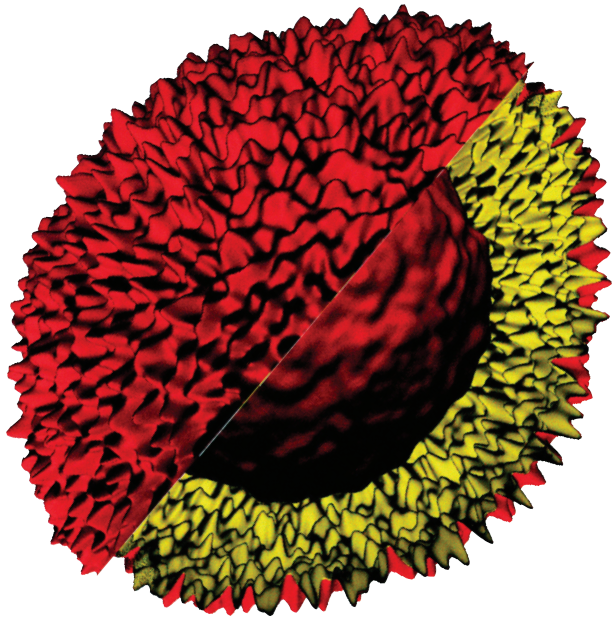
Developed by physicists Andrew Cook and Bill Cabot, MIRANDA can run as either a direct numerical simulation (DNS) or a large-eddy simulation (LES). In DNS mode, physical processes are calculated from first principles or as close as possible. In LES mode, models are added to describe some of the finer-scale physical processes and, thus, reduce the computational time.

"With this code, we can explore topics of interest, such as Rayleigh–Taylor instabilities and shock-induced mixing, at higher resolutions than ever before," says Livermore physicist Paul Miller. For instance, a high-resolution simulation of Rayleigh–Taylor instability revealed how the flow evolves through four stages. MIRANDA can even model the stage beyond the mixing transition, where the quantity of mixed fluid increases dramatically.

MIRANDA simulations are also allowing physicists to examine situations that are difficult to measure in experiments, such as fluid flow at high Reynolds numbers. The Reynolds number is a dimensionless parameter used to characterize the ratio of inertial effects to viscous effects in fluid flow. Flows at low Reynolds numbers are slow, small in size, viscous, or a combination of all three—for example, a raindrop sliding down a window, liquid being slowly sipped through a straw, or motor oil being poured from a container. Because these low-Reynolds-number flows involve a small range of scales, they are relatively easy to simulate.

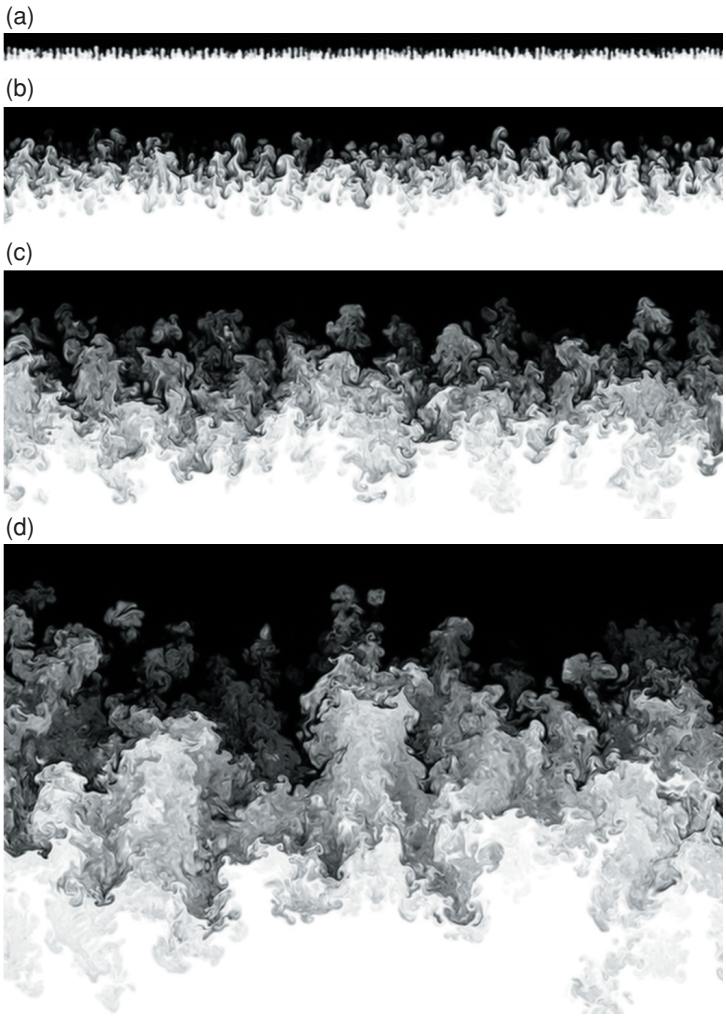
In contrast, flows at high Reynolds numbers are fast, large scale, less viscous, or some combination of those properties. High-Reynolds-number flows include air flowing around a truck on a freeway, swirling inside a thunderstorm, or jetting from the nozzle of a leaf blower. Such high-speed fluid dynamics are frequently of interest for scientific applications but are more challenging to compute.

By running MIRANDA in both DNS and LES modes, physicists can examine fluid dynamics at a wider range of Reynolds numbers. "With DNS techniques, we can only model flows at Reynolds numbers up to about 5,500," says Cook. "But with LES techniques, we can look at systems up to about 40,000." At these conditions,



These density isosurfaces from a HYDRA simulation of a NIF ignition capsule show the irregularities that result from Rayleigh–Taylor instabilities. The outer surface is near the ablator–fuel interface, and the inner surface is in the deuterium–tritium fuel. At 140 picoseconds before ignition time, the ignition capsule has a density of 60 grams per cubic centimeter and a diameter of 100 micrometers at maximum implosion velocity.

the simulations can only be validated by statistical comparisons with experiments, so the team is "bootstrapping" results. That is, they compare results generated at the limit of DNS techniques to those generated by LES. Agreement in the DNS and LES data helps them validate the LES results.



These vertical slices of density field from a three-dimensional simulation using the MIRANDA code illustrate the evolution of a Rayleigh–Taylor instability when two fluids with different densities are mixed. In this simulation, the heavier fluid is black. (a) Early on, the perturbations grow almost independently from one another. (b) Weak turbulence appears in the second stage when secondary Kelvin–Helmholtz instabilities appear. (c) The mixing transition occurring here results in more mixed fluid within the layer. (d) After the transition, mixing is enhanced, consistent with expected high-Reynolds-number behavior.

The runs are complex and use the tremendous computational resources of two Livermore supercomputers, MCR and ALC. In one calculation, 1,728 processors were used for nearly a month. When the BlueGene/L supercomputer is available, scientists will have the computing power needed to run DNS calculations above the mixing transition, an important regime in which to validate the LES results.

Bridging Fluid and Particle Motion

The CPK code, like HYDRA, can be applied to ICF problems. CPK's forte is semicollisional plasmas, where two fluids only partially collide. For example, when two puffs of gas are released, they "splash" into each other, and some—but not all—of their particles collide. Most of these particles flow in the same direction and at the same rate, near the average flow velocity. However, a few of them move in other directions, expanding away from the direction of flow and at significantly different velocities.

Although current simulation algorithms accurately model collisionless and collision-dominated plasmas, semicollisional plasmas have proven to be more difficult. "As it turns out, neither fluid nor kinetic models are adequate for the semicollisional regime," says Livermore scientist Dennis Hewett. "The simple hydrodynamics or fluid model assumes that the plasma is collision-dominated, and the velocity can be represented by a smooth Maxwellian distribution. However, because the hydrodynamics model doesn't look at the system particle by particle, it can't simulate ionization or particles that move against the flow."

A kinetic model, such as a particle-in-cell (PIC) code, performs calculations for "macroparticles," which are used to represent the system and thus capture the kinetic behavior of the system. "The drawback with a kinetic model is that macroparticles populate all of the areas—even those where nothing is going on that we're interested in," says Hewett, "and those calculations become expensive in terms of computational time and effort. Instead, what we need is an algorithm to bridge this gap by accurately simulating semicollisional systems."

The CPK code uses an ensemble of small, fluidlike macroparticles to represent particle distributions in phase space, a mathematical construct that has the number of dimensions needed to define the state of a given substance or system. These macroparticles are Gaussian-shaped in both position and velocity. That is, plots showing the position and velocity of the particles that comprise each macroparticle form a bell-shaped curve. As time progresses in the calculation, the internal dynamics of the macroparticles may cause their shape in phase space to "tilt" as the velocity and spatial distributions evolve. The macroparticles may then break apart or combine with other macroparticles as the simulation continues.

If a lot of kinetic activity emerges, the code allows one macroparticle to be fragmented into many smaller particles that can

be simulated with a kinetic model to make the important features easier to observe. Conversely, when collisions dominate a region with many macroparticles, those macroparticles can be merged, and their fluidlike behavior modeled with a hydrodynamics calculation. With this approach, computational effort is reserved for areas with the more relevant events and not squandered on less interesting areas. "The key to this approach," says Hewett, "is to design fragmentation and merging algorithms so that the code can reassemble the fragmented pieces and preserve the initial distribution without adding incidental new features or 'pseudo-physics' to the problem."

The CPK code works well at the limits of fluid and particle behavior. More importantly, results from semicollisional simulations, developed by coworker David Larson, agree with those from experiments, which helps validate the code's accuracy.

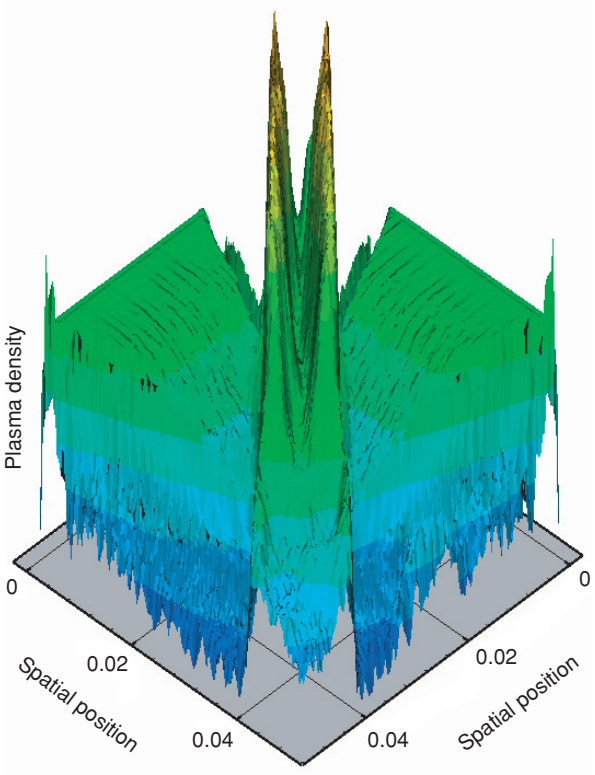
For example, Larson used CPK to simulate an experiment conducted by Livermore physicist Alan Wan in which a laser beam strikes two metal slabs, which are oriented 45 degrees from the beam and 90 degrees from each other. When the metal ionizes, two plasma beams stream off the surfaces and interpenetrate along the symmetry axis. Simulations performed with a fluid model do not allow interpenetration, so in those simulations, a strong density peak is formed where the two beams collide. This central peak eventually blows apart and forms two off-axis density peaks.

In the CPK simulation, the same general sequence evolves. However, because the beams initially interpenetrate instead of stagnating, the soft stagnation on-axis yields a significantly lower density. The subsequent off-axis density peaks are also lower than the peaks predicted by the fluid model. Results from the CPK simulations match the experimental results.

"We're now adding ionization physics to the code," says Hewett. "Livermore is one of the few places working on such a code to bridge fluid and collisionless models."

Just the Beginning

These three codes are not, of course, the only ones in AX Division's computational arsenal, says Rathkopf. There's RAPTOR, which like MIRANDA can be used to study hydrodynamic instabilities, but can adapt its underlying computational mesh in response to fluid conditions. LASNEX is a radiation and hydrodynamics code for ICF simulations. F3D models examine laser–plasma interactions, and KULL is a radiation and hydrodynamics code with similar capabilities to HYDRA.



Results from a simulation made with Livermore's CPK code show the plasma density that results from the interpenetration of two plasma beams. The leading edges of the beams are too low in density and moving too fast to collide appreciably. Thus, they interpenetrate to a significant degree. The CPK code efficiently models these dynamics by creating macroparticles that focus computational resources in areas of interest.

"We also have a suite of codes that we use to simulate the performance of a nuclear weapon's secondary stage," says Rathkopf. "Many of these codes have methods for simulating gas dynamics—exploring what happens when things are in motion."

—Ann Parker

Key Words: complex particle kinetics (CPK) code, high-energy-density physics, HYDRA code, hohlraum, hydrodynamics, MIRANDA code, plasma, Rayleigh–Taylor instability, Reynolds number.

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X Rays, Detonations, and Dead Zones

Livermore's high-flux radiography system can be used to image dynamic processes as they occur in metals, providing more detail on a material's strength and such mechanisms as spallation, fracture, and failure.

THE rapid, violent detonation of a high explosive (HE) generates supersonic shock waves that transfer energy by moving mass. According to Livermore physicist John Molitoris, trying to gather data on what happens to a material during this split second is often a case of "smoke and mirrors." He adds, "We hope the mirrors don't blow apart before the smoke ruins the view." But with the Laboratory's new high-flux radiography system (HFRS), the diagnostic capabilities for this harsh experimental environment have greatly improved.

The HFRS has no mirrors, and smoke is not a problem because the system can image right through it. Developed by a team of Livermore physicists, engineers, and technicians, the system combines 1-megaelectronvolt (MeV) and 450-kiloelectronvolt (keV) x rays to see clearly into the detonating material and examine the detonation as it twists, turns, and sometimes fails. The HFRS can provide a sequence of images showing a dynamic process as it occurs over time or a detailed three-dimensional (3D) reconstruction "snapshot" of images, all taken at the same time. The details revealed in these images are helping scientists better understand the physical processes in an HE detonation and in shocked materials.

Imaging the Tough Stuff

Molitoris first conceived of such a system about 5 years ago while conducting fragmentation experiments in Livermore's High Explosives Applications Facility (HEAF). "We were using HE detonations to investigate the dynamic failure of steel, watching cracks form and catching the resulting fragments," says Molitoris. "Catching the fragments is straightforward, but we needed radiography to observe the dynamics of crack formation and metal failure. The HEAF gun tank had a rudimentary x-ray capability, which we used for shadowgraphic imaging. By adding a 450-keV x-ray system in the tank, we started to develop a more powerful radiography system."

X-ray images taken with this new setup provided much more detail on the hydrodynamic processes. "We could distinguish shock waves formed from detonating HE and even the detonation front inside the steel pipe," says Molitoris. "When I saw these first images, I knew we had the beginnings of a powerful diagnostic tool."

A pilot system was developed in the HEAF gun tank to test different concepts for the final HFRS. With support from the Laboratory Directed Research and Development (LDRD) Program and later the Defense and Nuclear Technologies Directorate, Molitoris assembled the technical team for the HFRS project.

Bill Gilliam and Larry Crouch from DNT set up the facility operations. Installation in the HEAF firing tanks was facilitated by Ernie Urquidez and Pat McMaster, also of DNT. Engineering's Jan Batteux, Hank Andreski, Jim Travis, Brad Bratton, Gurcharn Dhillon, Gary Steinhour, and Rick Palmer designed and implemented both phases of the system. Chuck Cook from DNT was the radiographer, and scientist Raul Garza helped design and carry out the experimental program.

In the first test of the HFRS, Molitoris and his team received LDRD funding to explore the regime of warm, dense matter. Because this regime marks the transition between solids and plasmas, it is a particularly difficult region for recording experimental data. Thus, to evaluate the new system, the Livermore team used the HFRS to image shock waves in aerogels.

"We learned a lot about warm, dense matter and x-ray systems," says Molitoris, "and eventually outgrew the gun tank. This past year, we assembled the present HFRS in the HEAF spherical firing tank, which has more surrounding room and access ports. Now, we can combine dynamic x-ray imaging with diagnostics such as fast framing cameras, spectroscopy, velocimetry, and embedded fibers—all of which provide even more detail on the experiments."

The current HFRS uses two 1-MeV x-ray sources and two 450-keV sources to image detonations and shock waves in materials as diverse as aerogels and tantalum. The four sources were modified to produce higher currents and, thus, generate a higher flux of x rays. The HFRS is designed so that x-ray sources can be arranged in different experimental setups and triggered independently. For example, x-ray flashes can be staggered over time, as in a short movie, to provide a sequence of images that show a process as it evolves. Pulses also can be fired simultaneously, producing images that can be combined for 3D reconstruction of a dynamic process.

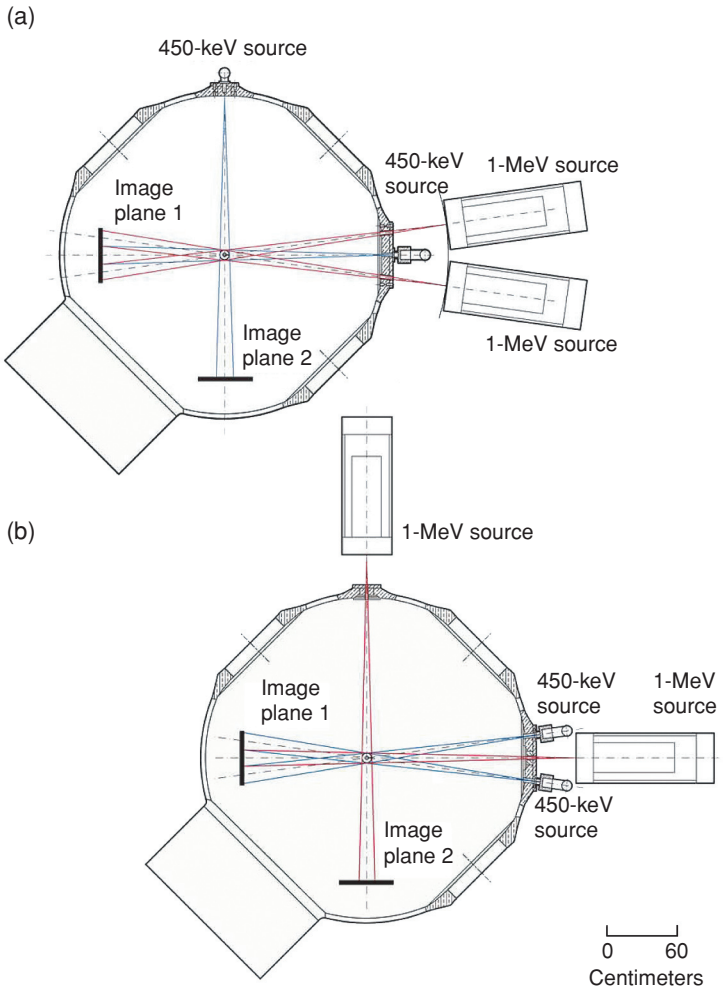
The team is considering other options for viewing the data in 3D. "We're working with physicist Maurice Aufderheide to explore a configuration that will act like a pair of eyes and produce stereoscopic images," says Molitoris. "Stereoscopic images can help us determine, for example, which side of a cylinder is fragmenting during detonation. Without the 3D aspect, we can't tell whether the near wall or the far wall is breaking up."

With the system's 25-nanosecond time resolution and 0.1-millimeter spatial resolution, scientists are imaging details never before seen in the detonation process. Recent experiments conducted with chemist Clark Souers focused on observing what happens when detonation propagates around a corner. "Understanding detonation propagation around corners and in even more complex geometries is vital for our stockpile stewardship work," says Molitoris.

In these experiments, a hemispherically shaped detonator is mated to a hemispherically shaped booster of the high explosive TATB. This piece is then placed in a well inside a cylinder of the high explosive LX-17, so that the cylindrical wall of LX-17 is above the TATB. When the TATB detonates, the detonation propagates hemispherically into the LX-17. Theory dictates—and code simulations indicate—that the detonation and its accompanying shock wave will "turn the corner" and continue up the wall of LX-17.

Reality, however, turned out to be quite different.

A time sequence taken with the HFRS shows that the detonation begins to fail as it hits the corner, and it continues to fail as it moves through the upper wall of LX-17. A region of nonreacting material, called a dead zone, forms as the shock front separates



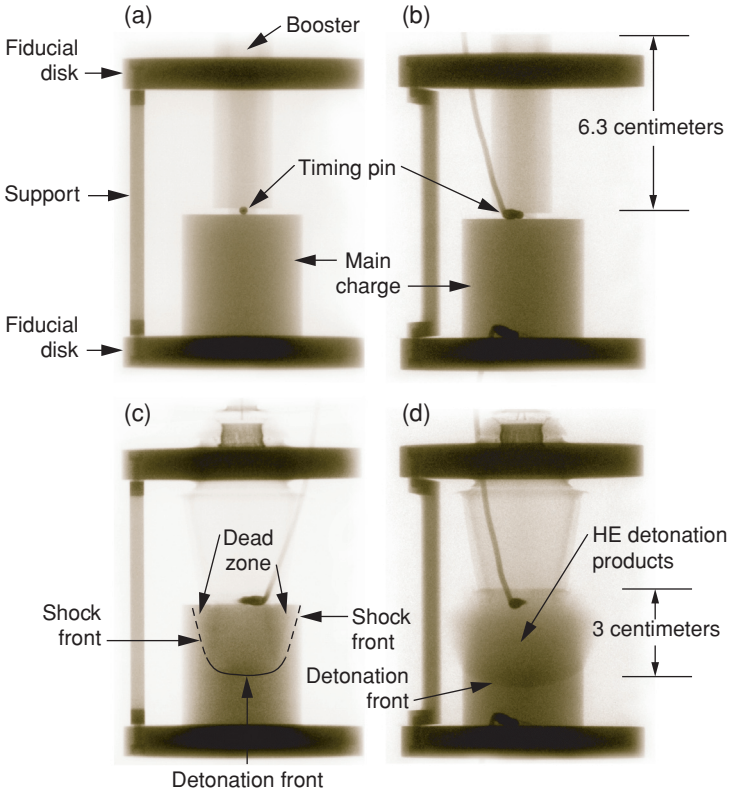
The x-ray sources on Livermore's high-flux radiography system can be moved to different positions. Two experimental setups for the 450-kiloelectronvolt (keV) and 1-megaelectronvolt (MeV) sources are shown in (a) and (b). X-ray sources also can be set up to trigger independently, which provides a sequence of images over time, or simultaneously, so the images can be combined in a three-dimensional reconstruction of a dynamic process.

from the dying detonation. As the detonation front moves farther from the corner, it begins to propagate through the upper wall of LX-17, leaving behind the doughnut-shaped dead zone.

"The formation of a long-lasting dead zone was totally unexpected," says Molitoris. "Results such as these—which are not anticipated by theory—demonstrate why new diagnostics such as the HFRS and the resulting experimental data are important."

But what is it about turning a corner that causes a dead zone to form? "We don't exactly know," says Molitoris. "The discontinuity, the corner in this experiment, initiates the dead zone, but its formation is also affected by the type of HE used. More ideal energetic materials can turn corners quite well, but not TATB-based materials such as LX-17."

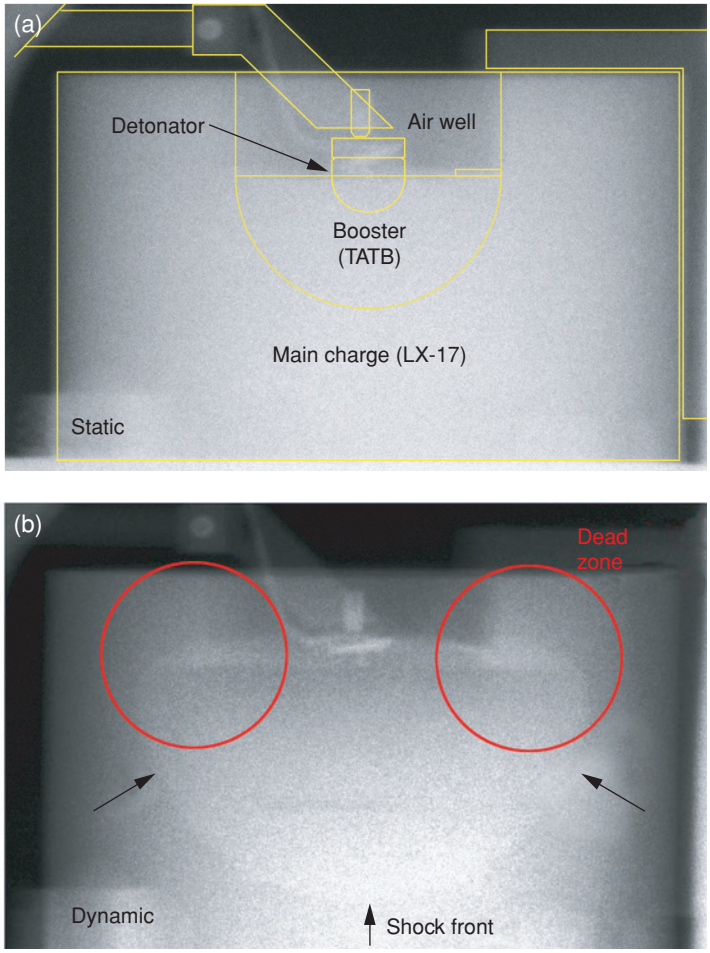
Experiments are helping the team study this phenomenon. "For instance, we're exploring whether temperature affects the size and structure of the dead zone," says Molitoris, "and we're examining other corner-turning geometries. All the information we gather will help us better understand the complex phenomenon of detonation. Modelers and theorists at Livermore need highly detailed data to improve the codes they're using in the Laboratory's stockpile stewardship work, so they can better predict detonation failure and quantify dead-zone formation."



Radiographs show the setup for detonation experiments using two high explosives (HE): (a) LX-17 and (b) LX-04. (c) After the detonation begins, LX-17 has a weak detonation front and forms a dead zone. (d) In the LX-04 experiment, the detonation front progresses vigorously through the main charge.

The Future Is Shocking

The HFRS continues to churn out intriguing data from various experiments, revealing previously unseen details about the nature of detonation. In what may be the first radiographic study of shock



A comparison of radiographs taken (a) before a high-explosive detonation and (b) 3.32 microseconds after the detonation starts to turn the corner shows regions of nonreacting material above the booster where detonation failed. These regions, or dead zones, persisted very late into the detonation process but were not predicted by theory or computer simulations.

behavior in aerogels, radiographic images of an LX-10 HE charge shocking silica aerogel clearly show the shock wave changing its shape as it propagates through the aerogel. "Once the shock wave hit the aerogel and was no longer supported by the detonation, the flat top of the shock front began to curve and broaden in the aerogel," says Molitoris. "With the earlier version of HFRS, we could almost see the Richtmyer–Meshkov mix structure in the transmitted shock. Our present system should be powerful enough to show those details."

The team is also exploring the difference in detonation and initiation in ideal and nonideal HE. In other experiments, the team is using the HFRS to measure the density variations that occur in metals shocked by a detonation, which will provide data on the viscosity of metals under dynamic loading. "It's been said that Lawrence Livermore is one of the few places that treats steel as a fluid," says Molitoris. "Up to now, our imaging capabilities did not provide enough detail inside the metal for us to quantify the density changes caused by shock loading. With HFRS, we can see those details, and we're now planning more difficult experiments with shocked metals."

The team also wants to investigate the process of deflagration in HE. Deflagration is a rapid chemical reaction that can quickly create heat, flame, sparks, or burning particles. Deflagrations generate separate subsonic pressure or shock waves instead of the mass flow of supersonic compression waves generated in HE detonations. As a result, the force of the expanding gas can be used to move an object—a bullet in a gun or a piston in an engine. In theory, deflagration is a slower process than detonation, and it can evolve into detonation. However, says Molitoris, "No one has ever been able to image that transition—up to now."

The HFRS is now operational and producing a wealth of information on material response to shock waves, detonation, and related hydrodynamic processes. The spherical firing tank at HEAF can handle up to 10 kilograms of (TNT-equivalent) HE, so it is ideal for relatively low-cost, focused experiments. The Department of Defense is interested in HFRS experiments to quantify mechanisms such as spallation, fracture, and failure. The team could also use the system to examine the detonation process in new advanced energetic materials that are being developed.

The Livermore team responsible for the high-flux radiography system is assembled between the 1-megaelectronvolt pulsers and the firing tank (from left): Hank Andreski, Sabrina Fletcher, Bradley Wong, Raul Garza, Jan Batteux, John Molitoris, Jim Travis, Pat McMaster, Larry Crouch, Brad Bratton, and Chuck Cook.

However, Molitoris says, "Our primary commitment is to support the Laboratory's stockpile stewardship mission by better understanding dynamic processes in metals and the corner-turning process in detonations. With the HFRS, we are helping Livermore and HEAF maintain the lead in detonation science."

—Ann Parker

Key Words: aerogel, deflagration, detonation, High Explosives Applications Facility (HEAF), high-flux radiography system (HFRS), hydrodynamics, x rays.

For further information contact John Molitoris (925) 423-3496 (molitoris1@llnl.gov).

Each month in this space, we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Guided Acoustic Wave Inspection System

Diane J. Chinn
U.S. Patent 6,799,466 B2
October 5, 2004
A system for inspecting a conduit for undesirable characteristics has a transducer system that induces guided acoustic waves onto said conduit. The conduit has at least two sides, and the transducer system uses flexural modes of propagation to provide inspection using access from only the one side of the conduit. Cracking is detected with pulse-echo testing using one transducer to both send and receive the guided acoustic waves. Thinning is detected in through-transmission testing where one transducer sends and another transducer receives the guided acoustic waves.

High Power Density Solid Oxide Fuel Cells

Ai Quoc Pham, Robert S. Glass
U.S. Patent 6,803,141 B2
October 12, 2004
A method for producing ultrahigh-power-density solid oxide fuel cells (SOFCs) involves the formation of a multilayer structure. A buffer layer of doped ceria is deposited between a zirconia electrolyte and a cobalt iron–based electrode using a colloidal spray deposition (CSD) technique. For example, a cobalt iron–based cathode may be deposited on a zirconia electrolyte via a buffer layer of doped ceria deposited by the CSD technique. These SOFCs have a power density of 1,400 megawatts per square centimeter (MW/cm^2) at 600°C and 900 MW/cm^2 at 700°C, which constitutes a power density two to three times greater than that produced by conventional SOFCs.

Wollaston Prism Phase-Stepping Point Diffraction Interferometer and Method

Michael C. Rushford
U.S. Patent 6,804,009 B2
October 12, 2004
This Wollaston prism phase-stepping point diffraction interferometer can be used as a test optic. The Wollaston prism shears light into reference and signal beams and provides phase stepping at increased accuracy by translating the Wollaston prism in a lateral direction with respect to the optical path. The reference beam produced by the Wollaston prism is directed through the pinhole of a diaphragm to produce a perfect spherical reference wave. The reference wave is then recombined with the signal beam to produce an interference fringe pattern of greater accuracy.

Optical Chirped Beam Amplification and Propagation

Christopher P. J. Barty
U.S. Patent 6,804,045 B2
October 12, 2004
This short-pulse laser system uses dispersive optics in a chirped-beam amplification architecture to produce high peak power pulses and high peak intensities. It also eliminates the potential for intensity-dependent damage to downstream optical components after amplification.

Awards

Livermore astrophysicist **Claire Max** is one of seven scientists to win the **Department of Energy**'s (DOE's) **2004 E. O. Lawrence Award**. The award is given for outstanding contributions in the field of atomic energy. Max received the award in the physics category for her contributions to the theory of laser guide star adaptive optics and its application to correct the blurring in astronomical images taken with ground-based telescopes. Max was the founding director of the Laboratory's Institute for Geophysics and Planetary Physics and continues to serve on that staff. In addition, she is a professor at the University of California (UC) at Santa Cruz and serves as deputy director for the university's Center for Adaptive Optics. Max is the 25th Livermore employee to receive the Lawrence Award since 1959, when it was established in memory of Laboratory cofounder Ernest Orlando Lawrence.

Two Livermore research collaborators, **Brian Wirth** and **Catherine Snelson**, were among a group of young scientists honored at a White House ceremony with the **2003 Presidential Early Career Award for Scientists and Engineers** (PECASE). Wirth and Snelson were nominated by the Laboratory for their collaborative research in support of DOE Defense Programs. They also received the **DOE Defense Programs Early Career Scientist and Engineer Award**. Wirth, a faculty member at UC Berkeley, received the awards for his work in computational dynamics studies of dislocations and defects in metals. Before joining UC Berkeley, he worked in Livermore's Chemistry and Materials Science Directorate. Snelson, who is with the University of Nevada at Las Vegas, was honored for her contributions in characterizing the geologic structure of the Las Vegas basin.

With support from Livermore's **Research Collaborations Program for Historically Black Colleges and Universities and Minority Institutions** (HBCUs and MIs), **Fisk University** in Nashville, Tennessee, received a **National Science Foundation Center of Excellence for Research in Science and Technology** (CREST) award to establish a Center for Physics and Chemistry of Materials. The Research Collaborations Program for HBCUs and MIs develops and promotes scientific connections between the Laboratory and universities that serve minority populations. The Laboratory's current collaborations with Fisk include studies of materials for solid-state tunable midinfrared lasers, radiation detectors for homeland security and space science applications, and an antifreeze protein found in arctic fish that prevents their blood from freezing in subzero temperatures.

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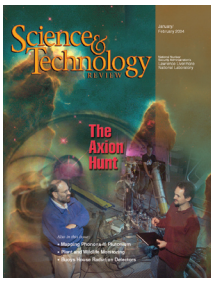

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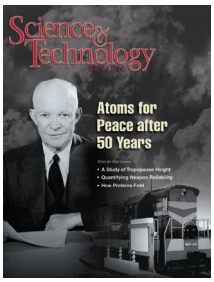

March 2004

April 2004

May 2004

June 2004

July/August 2004

September 2004

October 2004

November 2004

December 2004

Abstracts

Putting the Squeeze on Materials

Livermore physicists are using polished diamonds in opposing pairs, or anvils, to compress samples of materials at extreme pressures. This device, called a diamond anvil cell (DAC), forces materials to reveal new information about how their structure and electrical and magnetic properties change in response to increasing pressure. The researchers have taken advantage of recent improvements in diamond synthesis technology to fabricate microcircuits within the diamond anvils. The microcircuits, made from tungsten, serve as tiny diagnostic instruments to measure data about materials' fundamental physical and mechanical properties under high pressures. The modified diamonds, called designer diamond anvils, are used to learn how high pressures cause materials to change their magnetic properties, switch from insulators to metals, and alter their molecular structures. The Livermore team makes three types of designer diamond anvils: one for high-pressure electrical conductivity experiments, another for magnetic susceptibility experiments, and a third for electrically heating high-pressure samples to high temperatures. Each type features a unique pattern of microcircuits, which are fabricated on the diamond tip and then encapsulated within a diamond film.

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The Art of Protein Structure Prediction

The Protein Structure Prediction Center at Livermore brings together groups from around the world for the biennial Critical Assessment of Techniques for Protein Structure Prediction (CASP). Participants submit models of selected proteins, and independent assessors compare predictions to experimental results. CASP participants hope to develop computational techniques that, in conjunction with experimental methods, more rapidly determine protein structures. The Livermore center has created software that helps assessors evaluate models. Assessors also evaluate predictions from the growing number of automated servers that are being used for protein structure prediction. The Livermore team has begun creating a protein model database to promote the development of protein structure models and facilitate the ways the models can benefit other projects.

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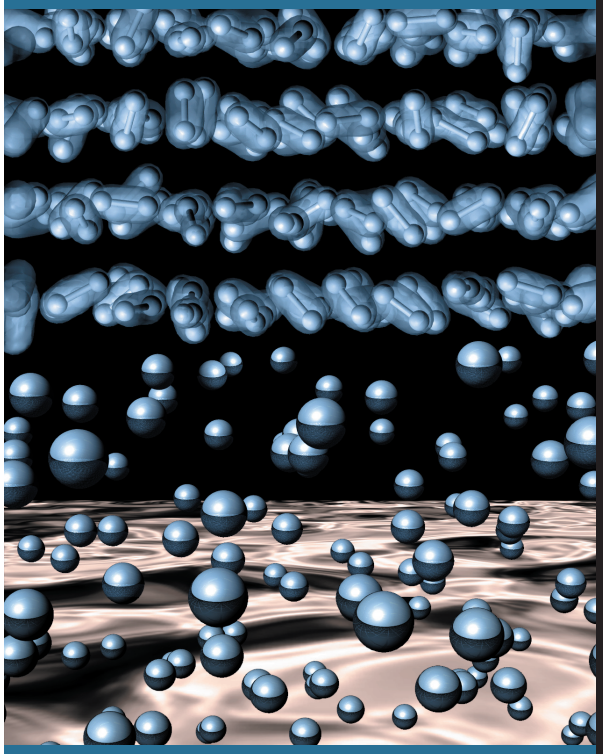
U.S. Government Printing Office: 2004/783-059-10002

Supercomputer Simulations Advance Science



Computer simulations have become powerful tools for understanding and predicting the physical universe, from the interactions of individual atoms to the details of climate change.

Also in January/February

- *A Department of Energy program is helping to develop nonweapons-related careers for Russian nuclear workers.*
- *Livermore's Terascale Simulation Facility is built to house almost half a petawatt of computing power and offers the flexibility to accommodate future computer systems.*
- *A Laboratory-developed technology allows geothermal power plants to "mine" valuable minerals from brines.*

Coming Next Month

University of California
Science & Technology Review
Lawrence Livermore National Laboratory
P.O. Box 808, L-664
Livermore, California 94551